



Development of NEMO 3-D: Numerical surface treatment for finite-extent semiconductor nanostructures

Gerhard Klimeck

Seungwon Lee, Fabiano Oyafuso, Timothy B. Boykin*,
R. Chris Bowen,, and Paul von Allmen

Jet Propulsion Laboratory, California Institute of Technology
University of Alabama in Huntsville

gekco@jpl.nasa.gov, 818-354-2182
<http://hpc.jpl.nasa.gov/PEP/gekco>

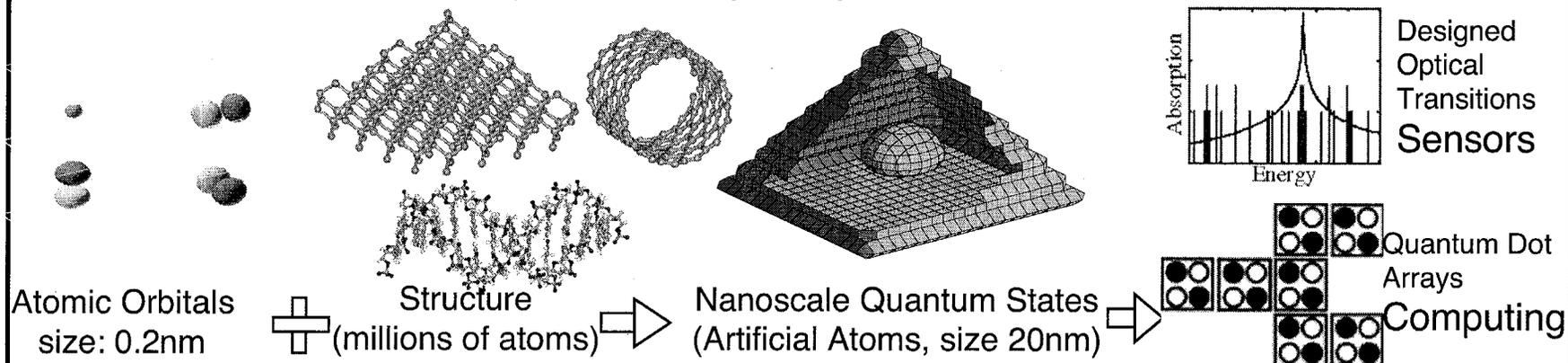
This research was carried out by at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration.

Outline

- **Motivation.**
- **High Performance Computing .**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations

Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin*, R. Chris Bowen, and Paul von Allmen



Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom => use pseudo-potential or local orbitals
- Consider finite extent, not infinitely periodic => local orbital approach
- Need at minimum one million atoms. => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape. => **need a design tool**

Approach:

- Leverage NEMO 1-D:
 - 25 person years at TI / Raytheon
 - 250,000 lines of code.
- Use local orbital description for individual atoms in arbitrary crystal / bonding conf.
 - Use s, p, and d orbitals
 - Use genetic algorithm for fitting
- Compute mechanical strain in the system.
- Develop parallel algorithms to generate eigenvalues/vectors of very large matrices ($N=3.2 \times 10^8$ for a 16 million atom system).
- Develop prototype GUI for (NEMO-3D)

Four Generations of Cluster Experience

Hyglac (1997)

16 Pentium Pros 200MHz
 128 MB RAM per node
2 GB total
 5GB Disc per node
80 GB total
 100 Mb/s ethernet crossbar
 Linux, MPI
 3.2GFlops

Nimrod (1999)

32 Pentium IIIs 450MHz
 512 MB RAM per node
16 GB total
 8GB Disc per node
256 GB total
 100 Mb/s ethernet crossbar
 Linux, MPI
 14.4 GFlops

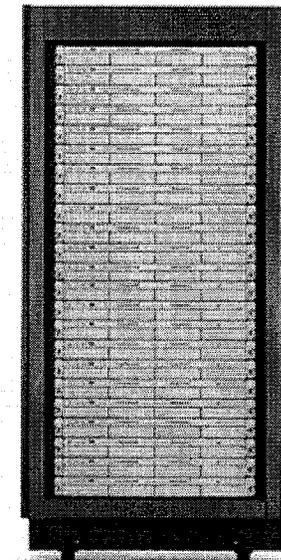
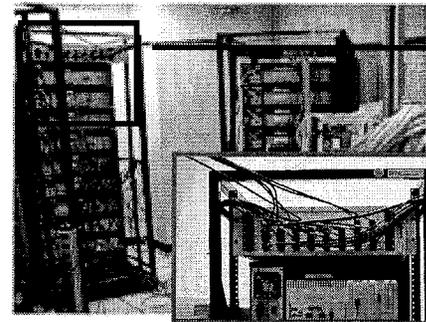
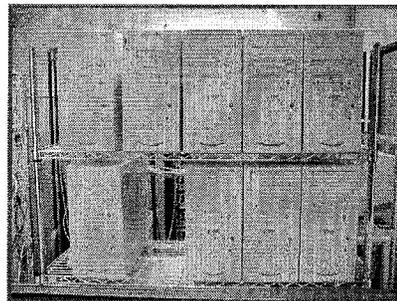
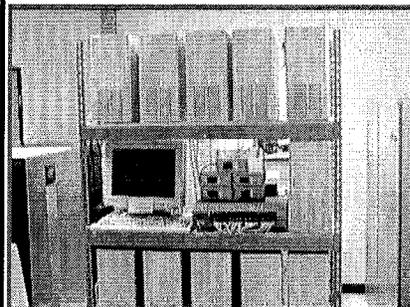
Pluto (2001)

64 Pentium IIIs
 800MHz
dual CPUs
 2 GB RAM per node
64 GB total
 10 GB Disc per node
320 GB total
 2 Gb/s Myricom crossbar
 Linux, MPI
 51.2 GFlops

NewYork (2002)

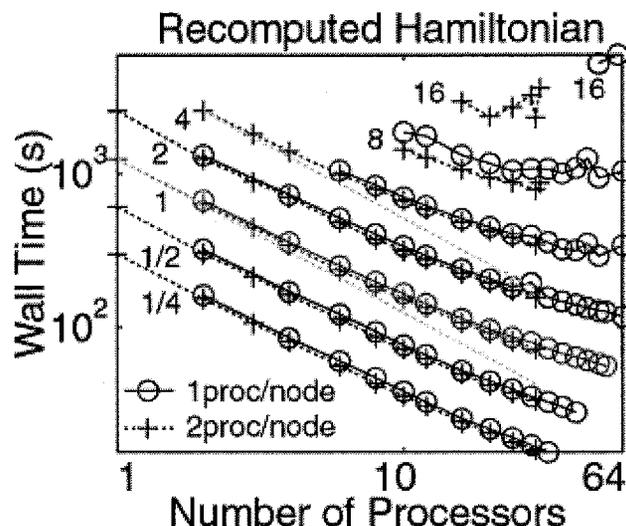
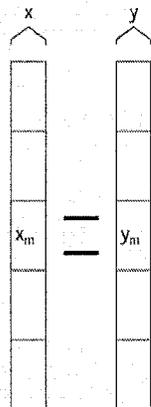
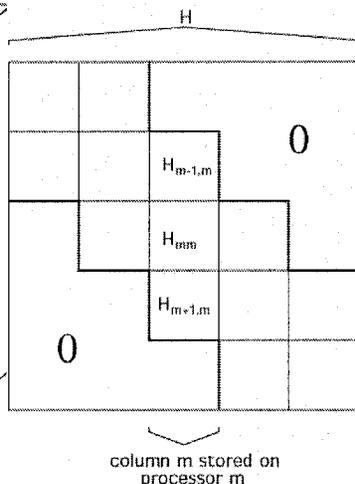
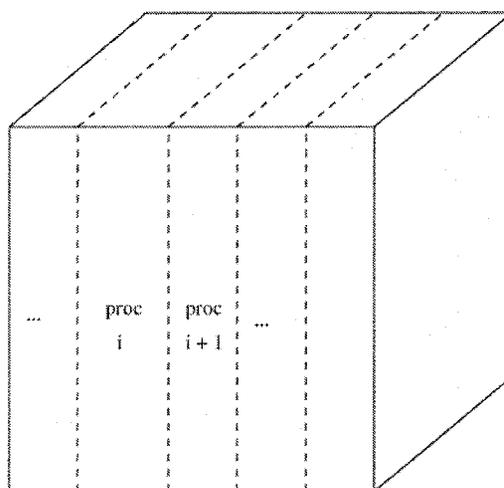
66 Xserve G4 1GHz
 1GB RAM per node
33 GB total
 60 GB Disc per node
2 TB total
 100 Mb/s ethernet crossbar
 MAC OS X, MPI
 495GFlops

Gordon Bell Prize 1997



Parallel Eigenvalue Solver on a Beowulf

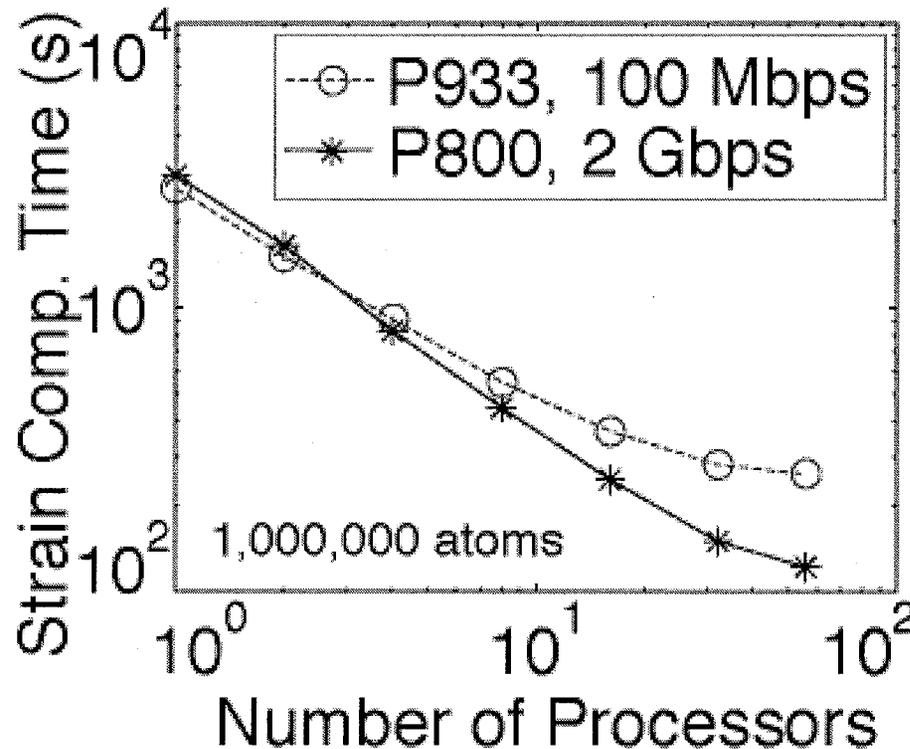
(32 node, dual CPU Pentium III, 800MHz, Linux)



- Divide Simulation domain into slices.
- Communication only from one slice to the next (nearest neighbor)
- Communication overhead across the surfaces of the slices.
- Limiting operation: sparse matrix-vector multiplication
- Enable Hamiltonian storage or re-computation on the fly.

- Systems from 1/4 to 16 million atoms
- sp3s* basis, Matrix sizes up to $1.6 \cdot 10^8 \times 1.6 \cdot 10^8$
- Large problems do not fit on one CPU
- Recompute Hamiltonian on the fly.
- Measure time for 30 Lanczos iterations
- 1million atoms 5000 iteration 1 CPU: ~48 hours 20 CPUs: ~3.4 hours
- Computation time linear in system size.

Parallelization of Strain Calculation



Problem (1million atoms):

- Serial strain computation:
~43 min.
- Serial electronic structure calculation (1000 iterations):
~ 9.6 hours
- Parallel electronic structure computation on 20 CPUs:
~41 min.

Solution:

- Parallelize strain calculation as well

Result:

- Reduce time to 2-5 minutes on a parallel machine.
- See difference between a fast 2Gbps and a 100Mbps network.
- Do not see that difference in the electronic structure calculation.
- Parallel strain computation is more communication dependent than the electronic structure calculation.

Outline

- **Motivation.**
- **High Performance Computing.**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Inhomogeneous Broadening due to Alloy Disorder

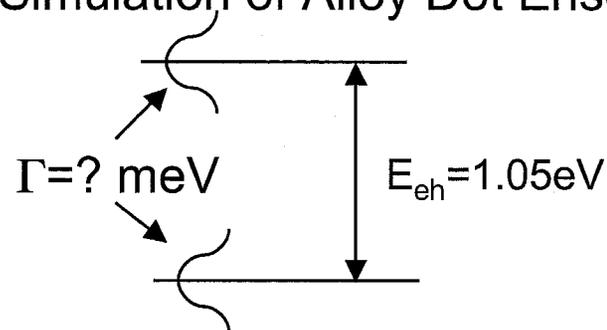
Problem:

- Cations are randomly distributed in alloy.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?
- Requires atomistic simulation tool.

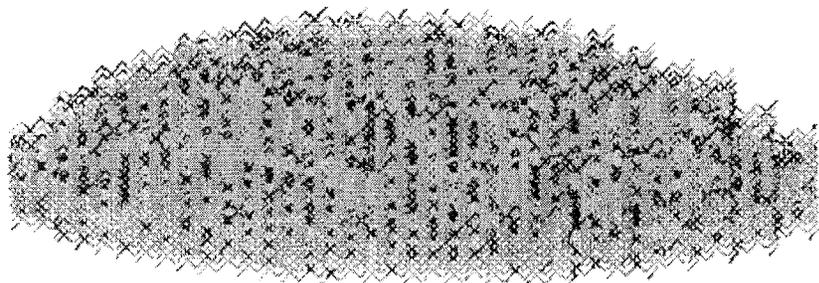
Approach:

- Simulate a statistical ensemble of dots.
 - Identical in size and shape
 - Different only in cation ordering.

Simulation of Alloy Dot Ensemble

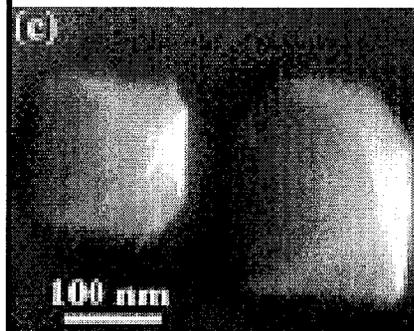


Measured $\Gamma=34.6$ meV (R. Leon, PRB, 58, R4262)



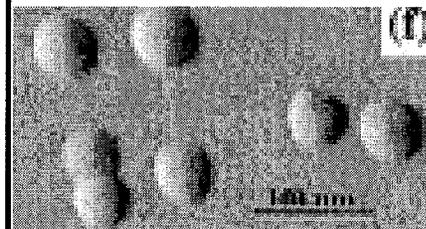
In_{0.6}Ga_{0.4}As Lens Shaped Dot

Diameter=30nm, Height=5nm, GaAs embedded
 ~1,000,000 Atom Simulation, sp³s* basis
 In and Ga atoms are randomly distributed
 Inhomogeneous Broadening?



**Quantum Dots:
 Self-assembled ,
 InAs on GaAs.**

**Pyramidal or
 dome
 shaped**



**R. Leon et al,
 JPL (1998)**

Inhomogeneous Broadening due to Alloy Disorder

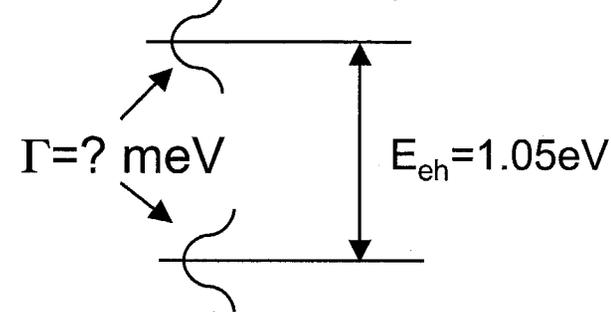
Problem:

- Cations are randomly distributed in alloy.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?
- Requires atomistic simulation tool.

Approach:

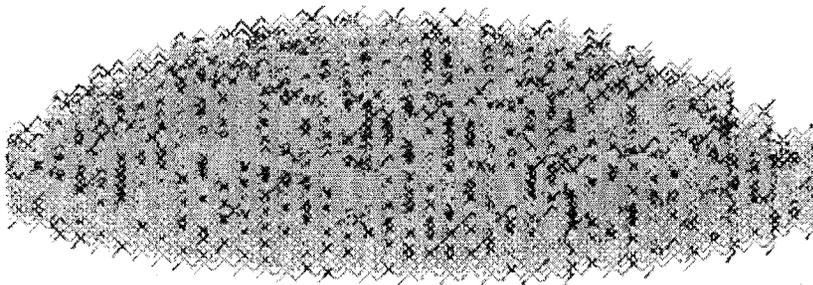
- Simulate a statistical ensemble of dots.
 - Identical in size and shape
 - Different only in cation ordering.

Simulation of Alloy Dot Ensemble



Measured $\Gamma = 34.6$ meV (R. Leon, PRB, **58**, R4262)

1~5meV Represents Theoretical Lower Limit

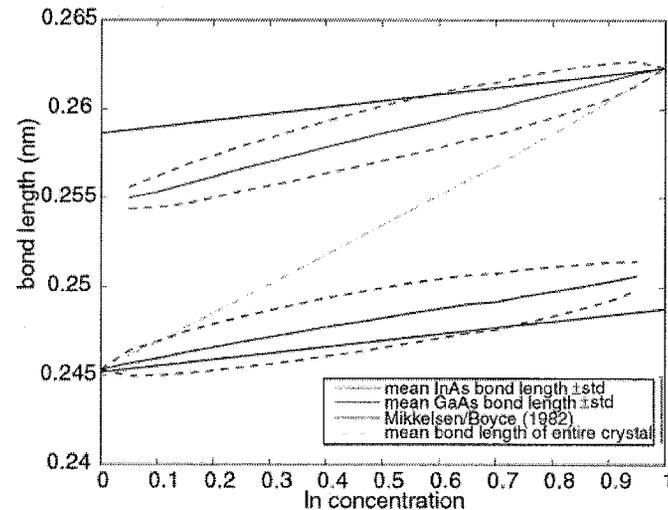


In_{0.6}Ga_{0.4}As Lens Shaped Dot

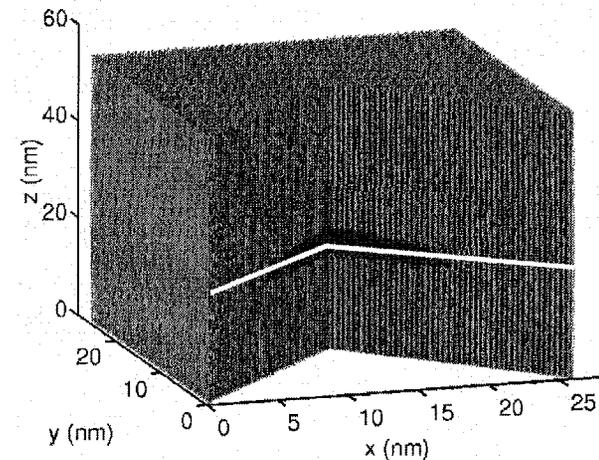
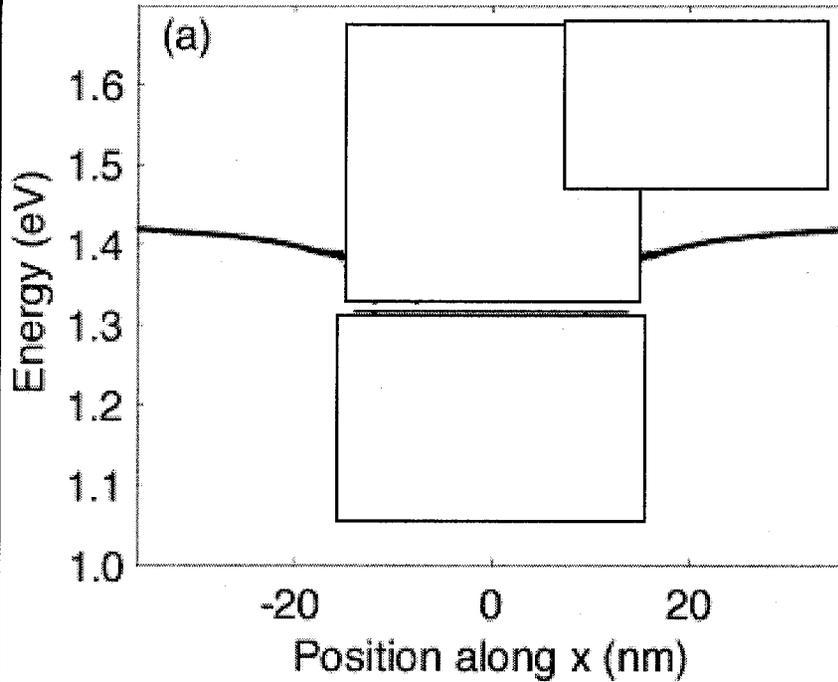
Diameter=30nm, Height=5nm, GaAs embedded
~1,000,000 Atom Simulation, sp³* basis

In and Ga atoms are randomly distributed
Inhomogeneous Broadening?

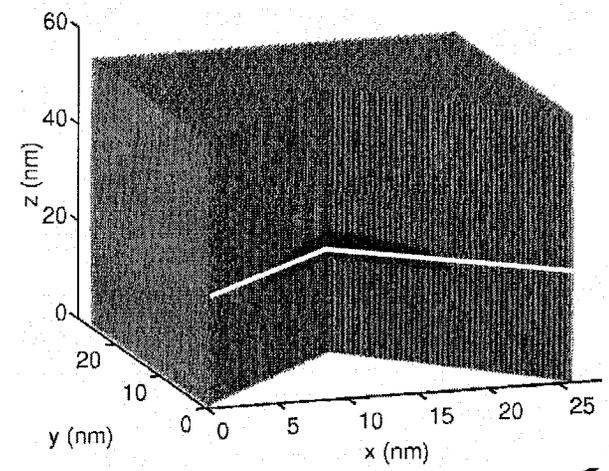
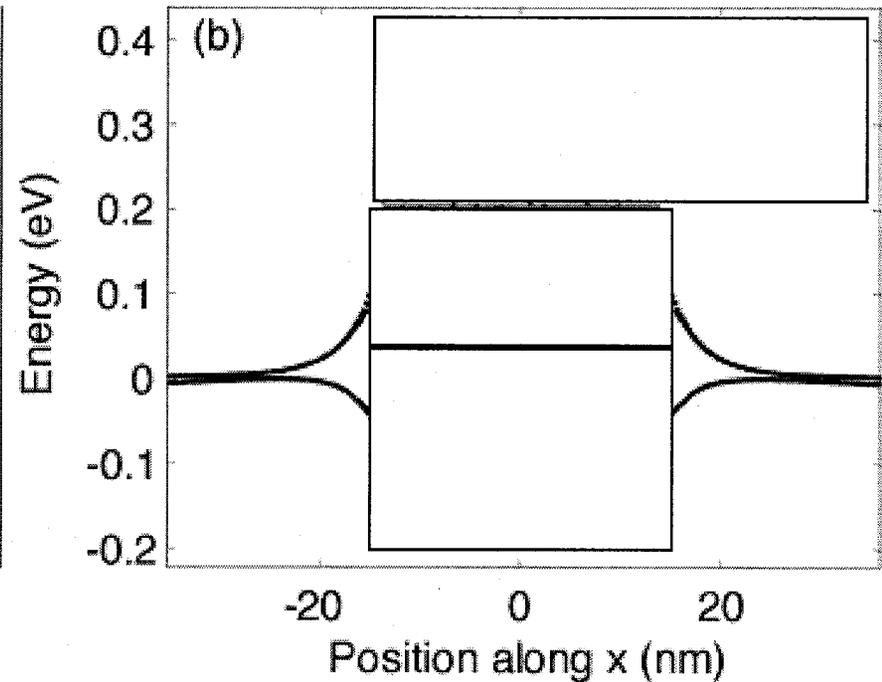
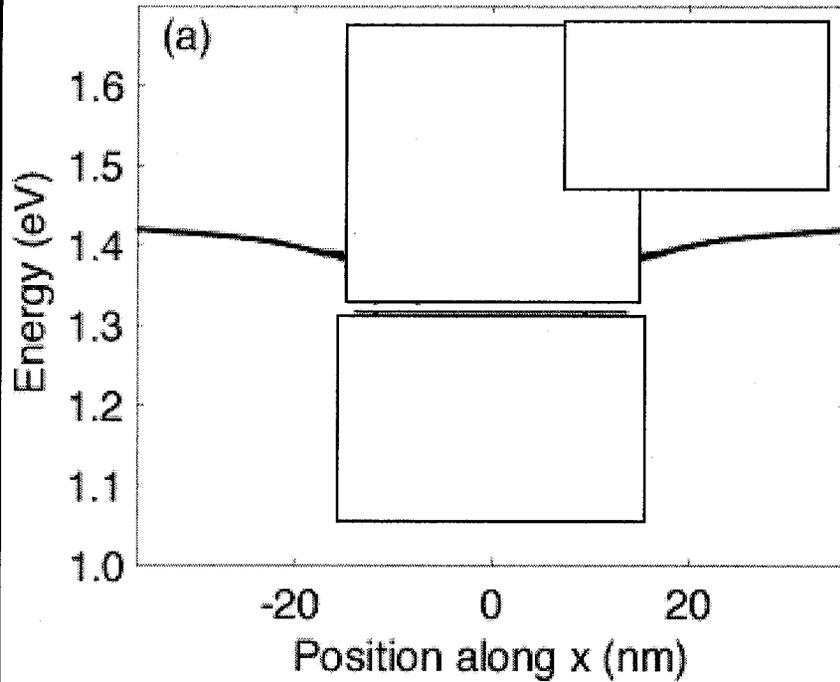
InGaAs has bi-modal bondlength distribution:
InAs-like and GaAs-like bonds!



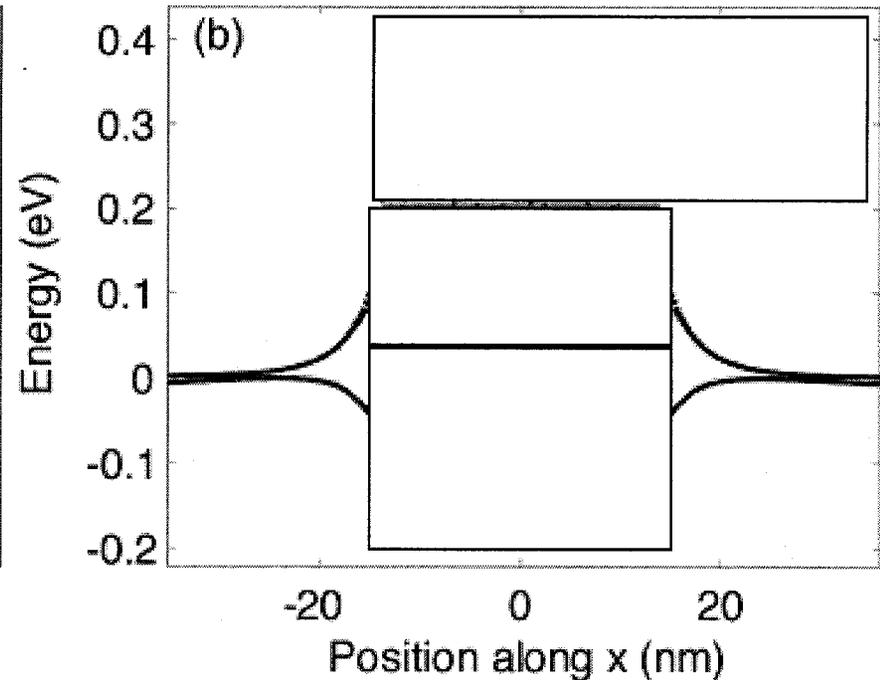
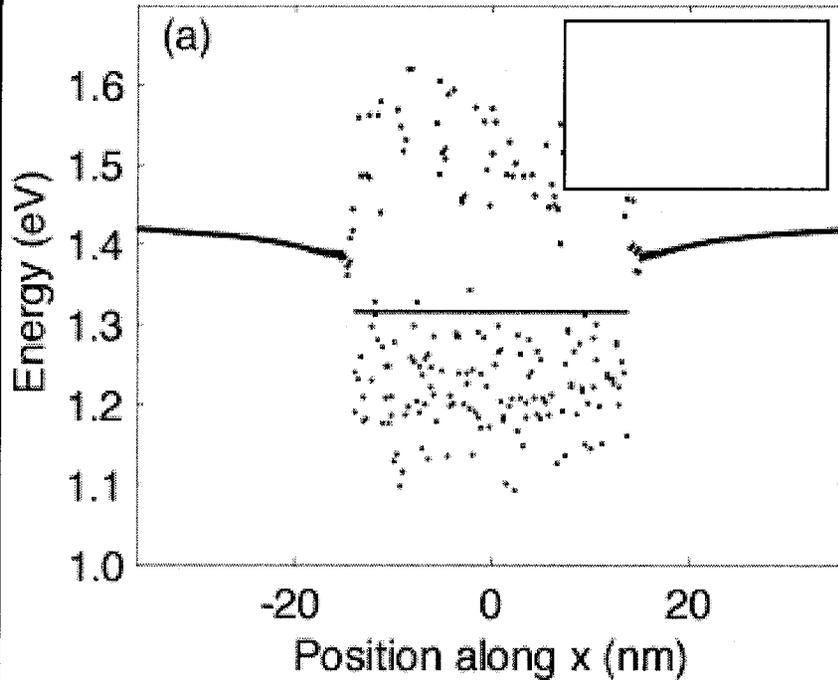
Local Bandstructure in an Alloyed QD



Local Bandstructure in an Alloyed QD



Local Bandstructure in an Alloyed QD

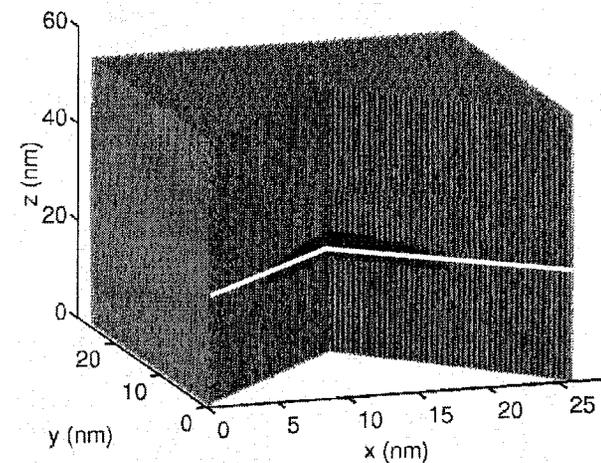


In-As bonds compressed in x-y

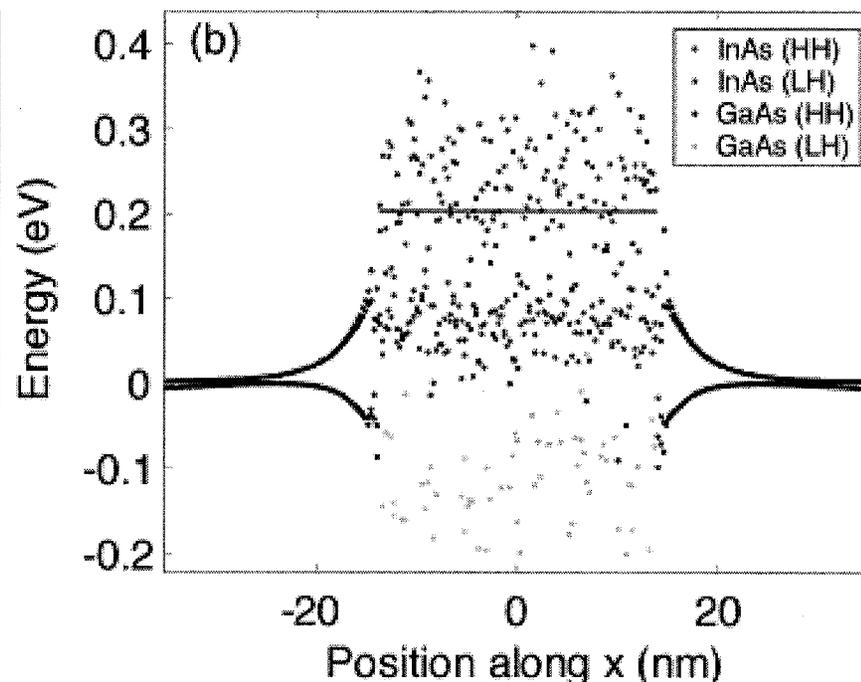
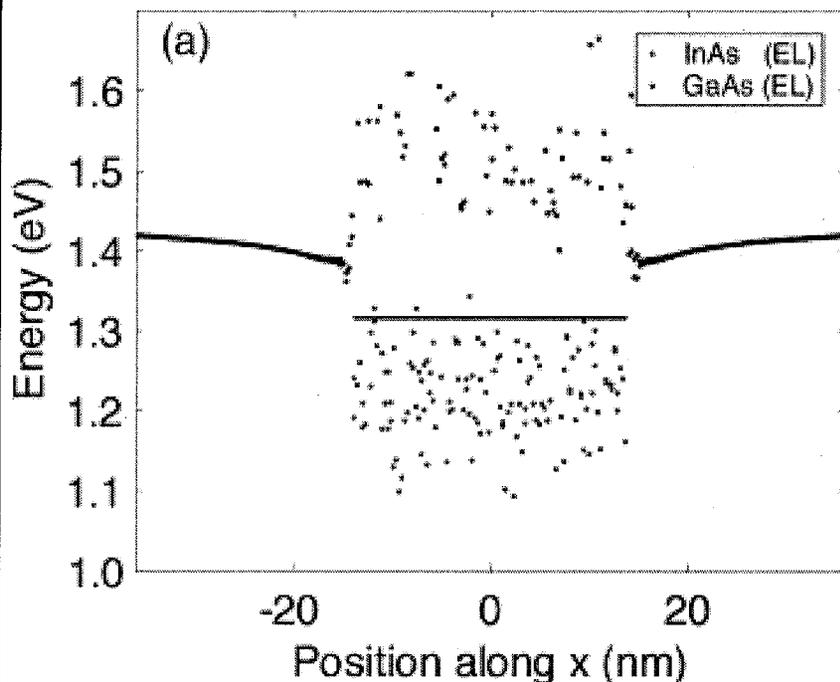
-> E_c raised from bulk value of $\sim 0.58\text{eV}$ to $\sim 1.2\text{eV}$

Ga-As bonds compressed in x-y and stretched in z

-> E_c raised from bulk value of $\sim 1.42\text{eV}$ to $\sim 1.55\text{eV}$



Local Bandstructure in an Alloyed QD

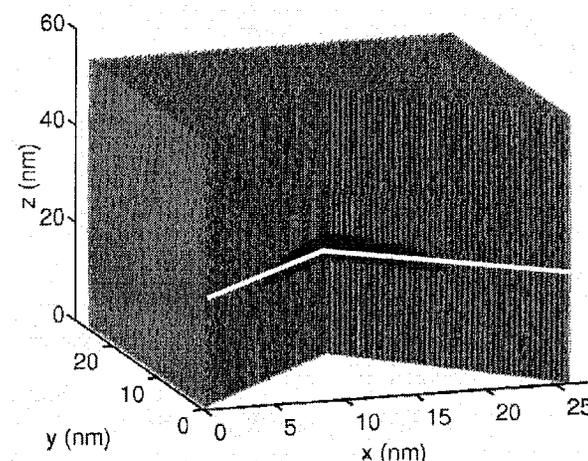


In-As bonds compressed in x-y

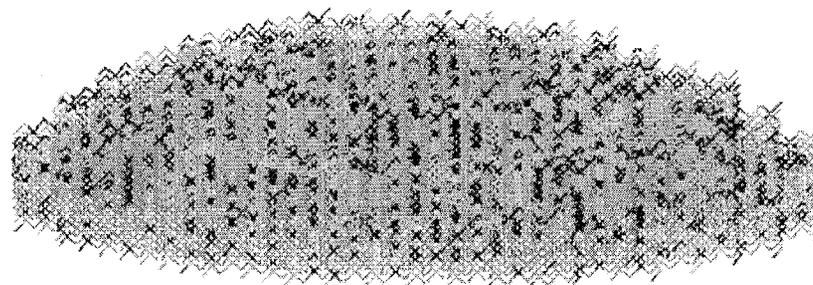
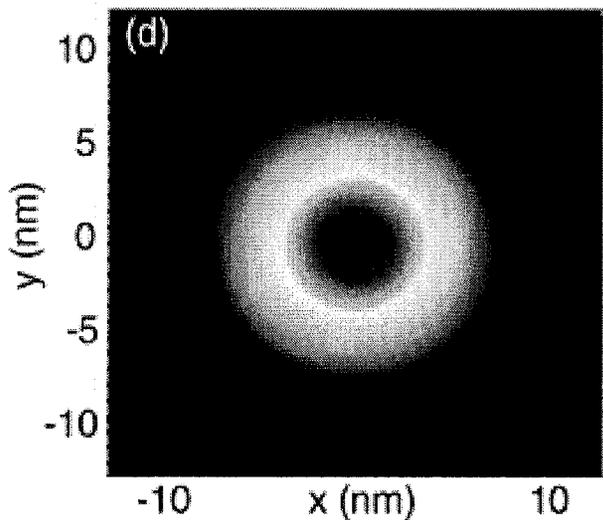
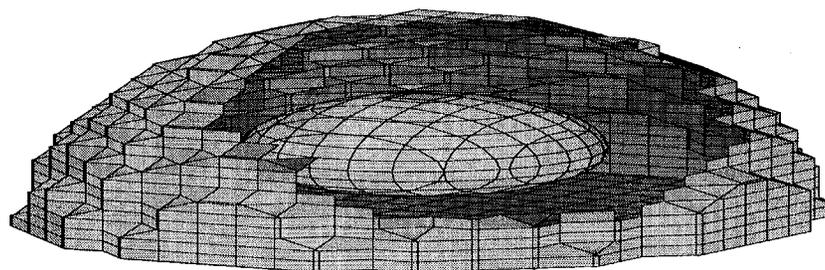
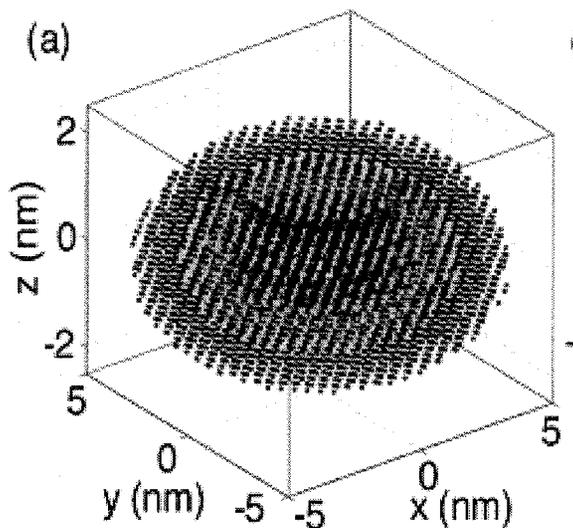
- > E_c raised from bulk value of $\sim 0.58\text{eV}$ to $\sim 1.2\text{eV}$
- > E_v HH raised from bulk value of $\sim 0.22\text{eV}$ to $\sim 0.3\text{eV}$

Ga-As bonds compressed in x-y and stretched in z

- > E_c raised from bulk value of $\sim 1.42\text{eV}$ to $\sim 1.55\text{eV}$
- > E_v raised from bulk value of 0eV to $\sim 0.1\text{eV}$

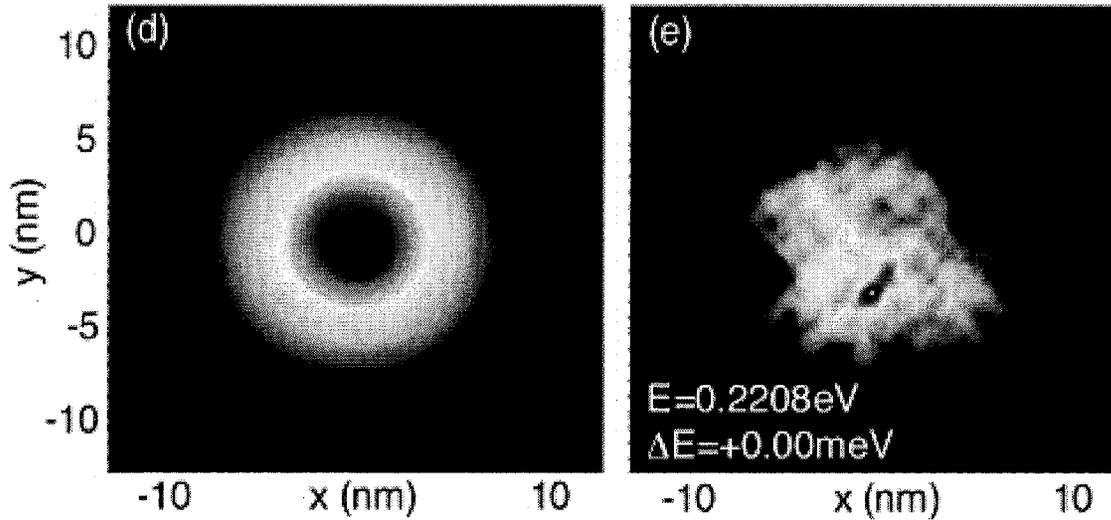
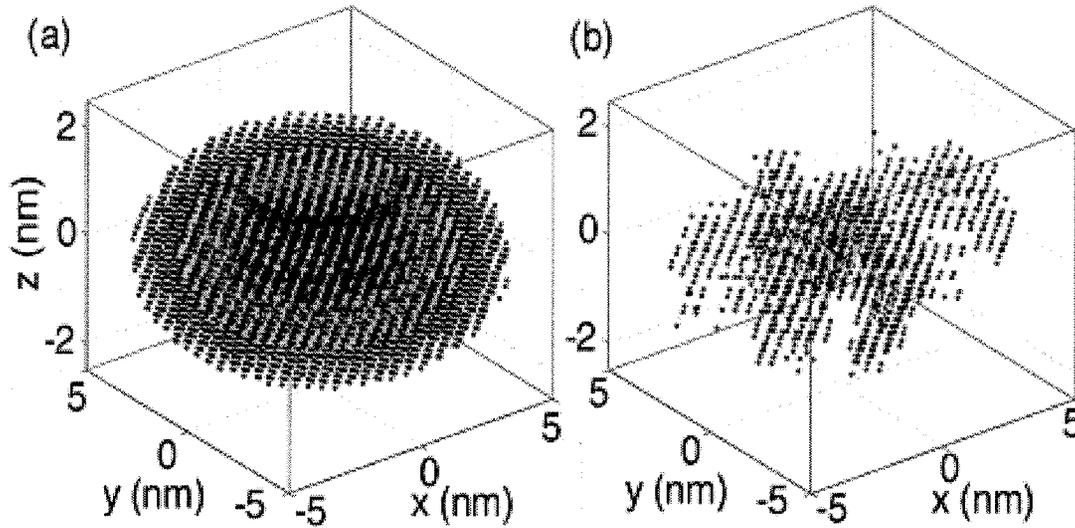


Spatial Irregularity in the Hole Ground State



VCA / no Disorder

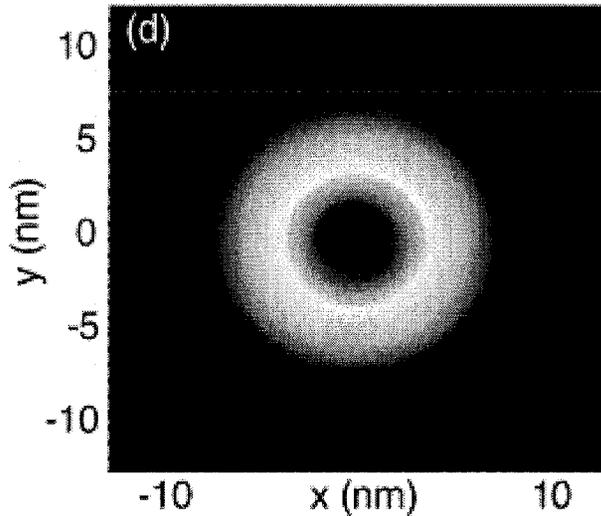
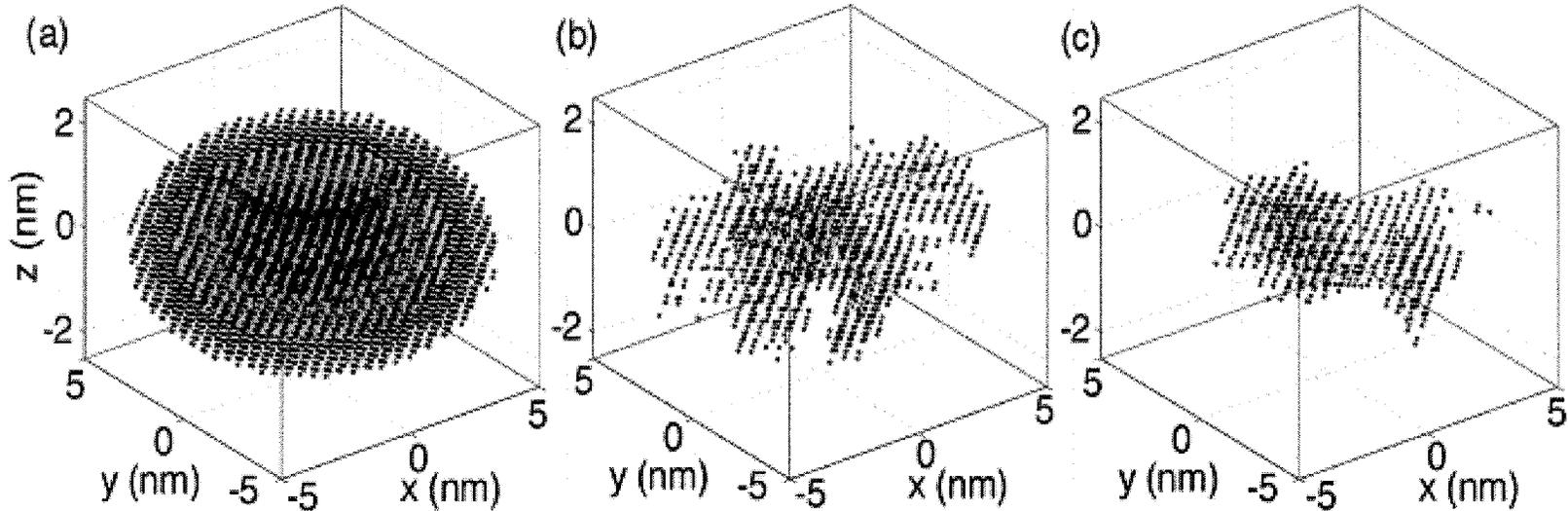
Spatial Irregularity in the Hole Ground State



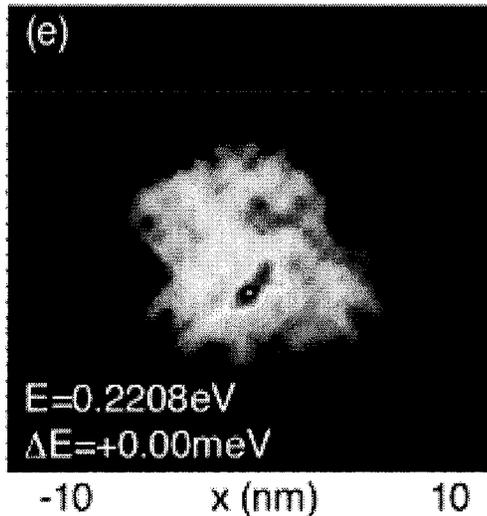
VCA / no Disorder

Disorder Sample

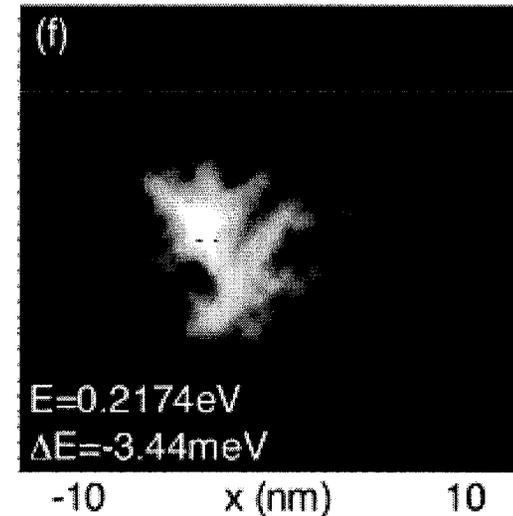
Spatial Irregularity in the Hole Ground State



VCA / no Disorder

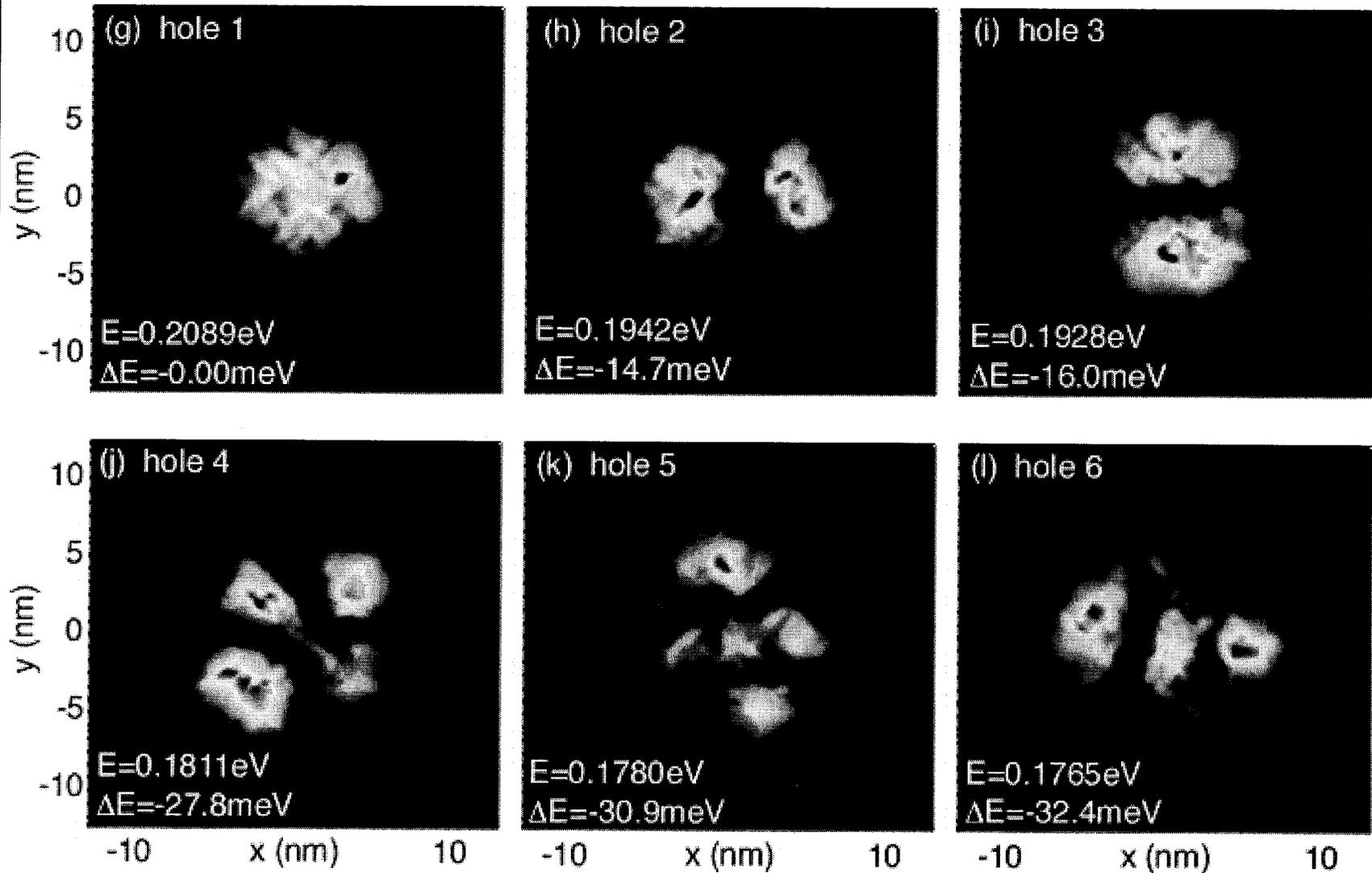


Disorder Sample 1

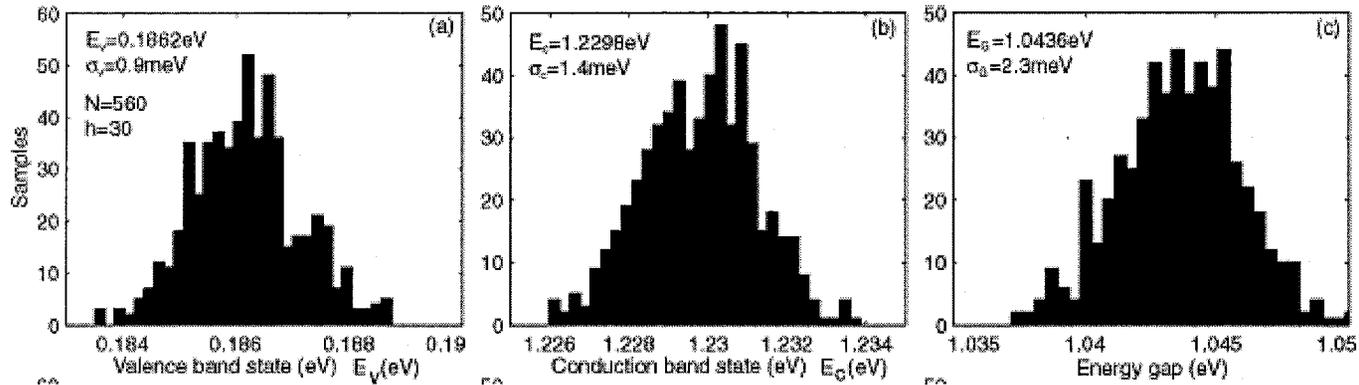


Disorder Sample 2

Spatial Irregularity in the Hole States

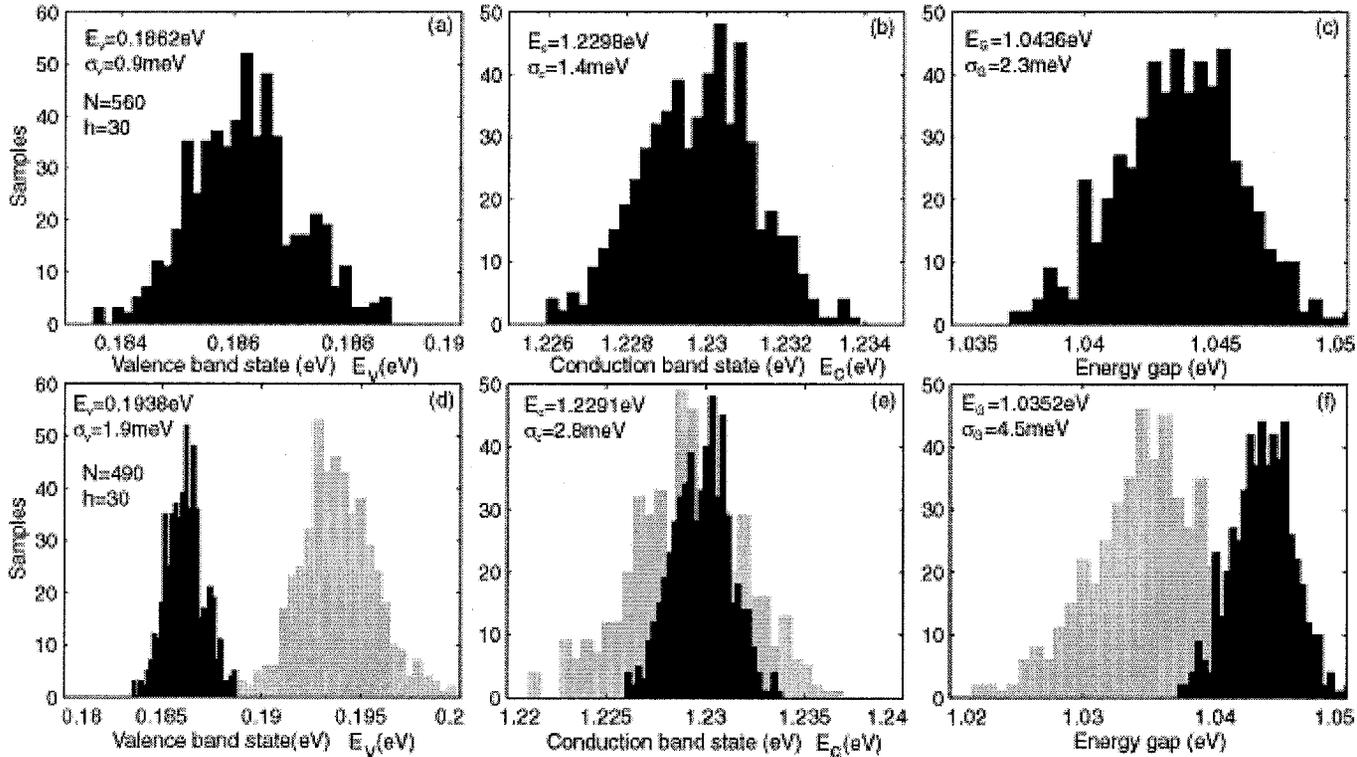


>1000 Alloyed Quantum Dot Samples



- Atomistic granularity
- $\sigma = 2.3$ meV

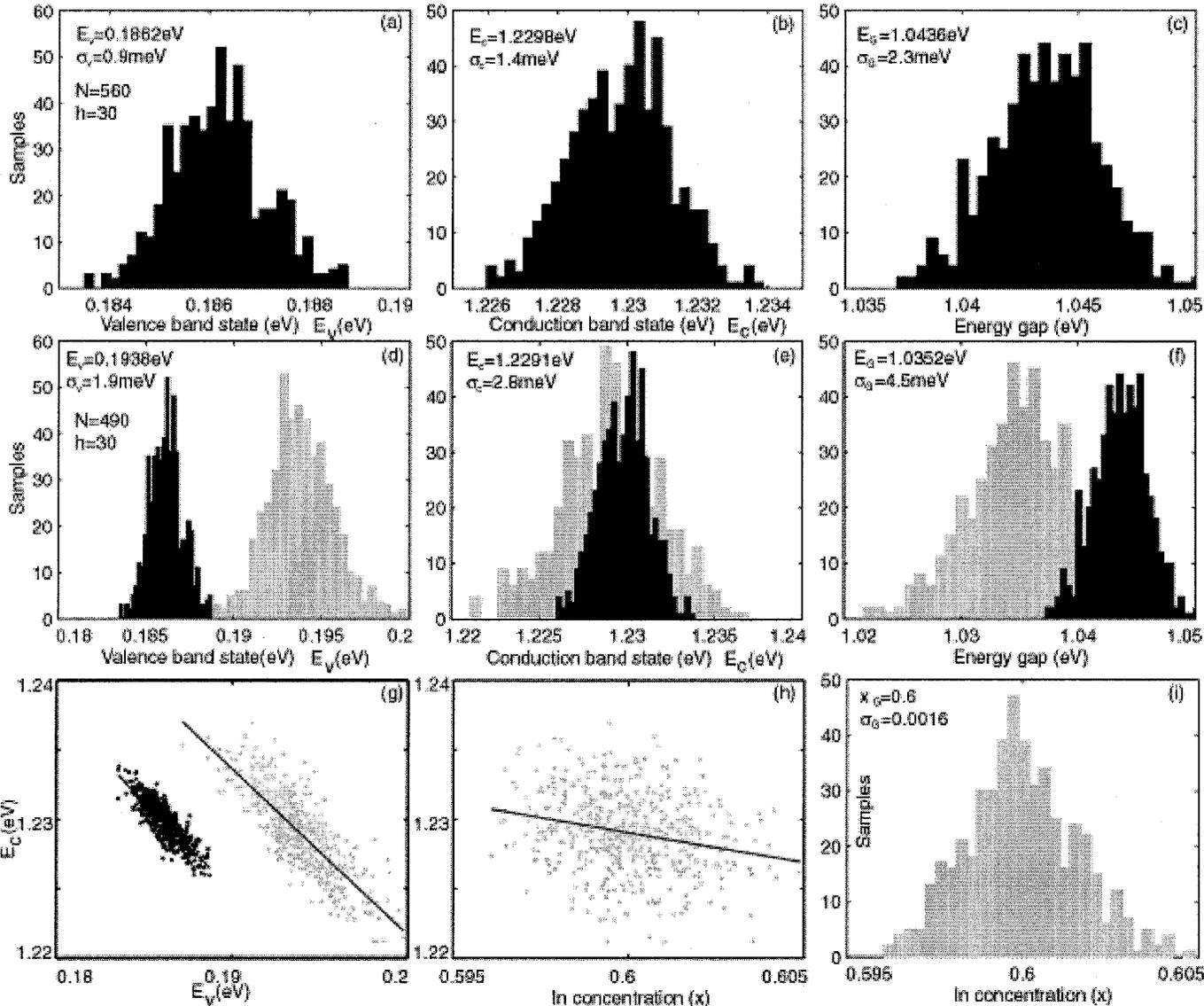
>1000 Alloyed Quantum Dot Samples



- Atomistic granularity
 $\sigma = 2.3$ meV

- Cell granularity
 $\sigma = 4.5$ meV

>1000 Alloyed Quantum Dot Samples

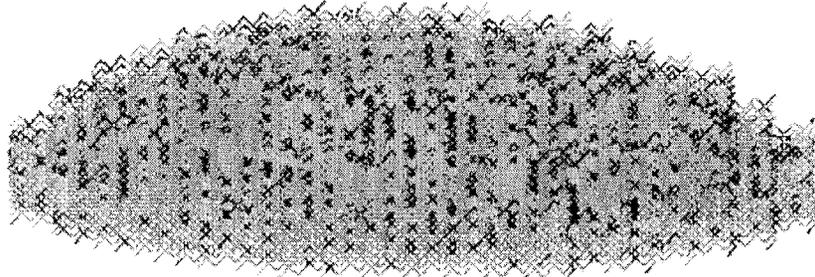


- Atomistic granularity
 $\sigma = 2.3\text{meV}$

- Cell granularity
 $\sigma = 4.5\text{meV}$

- E_c and E_v strongly correlated
- E_c and x weakly correlated

Inhomogeneous Broadening due to Alloy Disorder

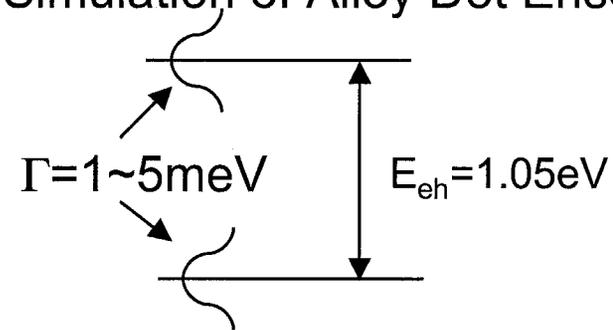


In_{0.6}Ga_{0.4}As Lens Shaped Dot

Diameter=30nm, Height=5nm, GaAs embedded
~1,000,000 Atom Simulation, sp3s* basis

In and Ga atoms are randomly distributed
Inhomogeneous Broadening?

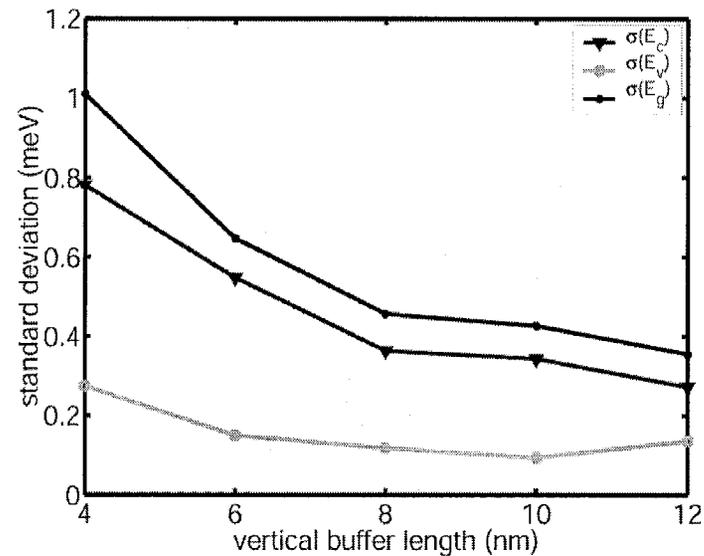
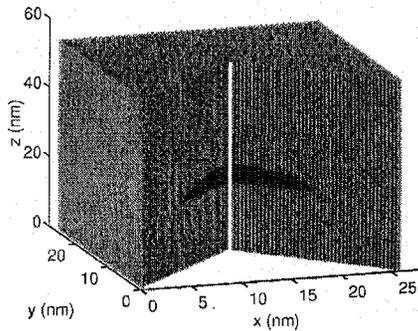
Simulation of Alloy Dot Ensemble



Measured $\Gamma = 34.6 \text{ meV}$ (R. Leon, PRB, **58**, R4262)

1~5meV Represents Theoretical Lower Limit

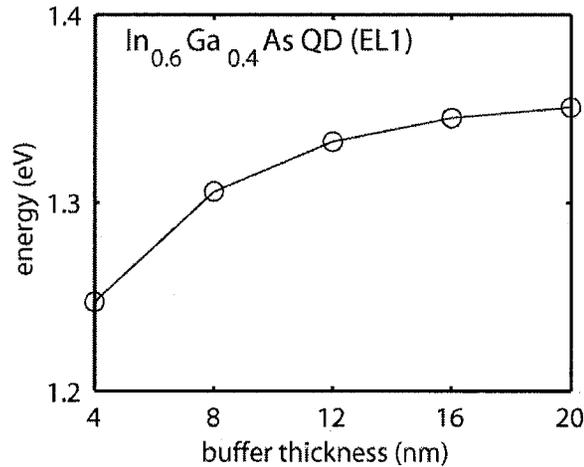
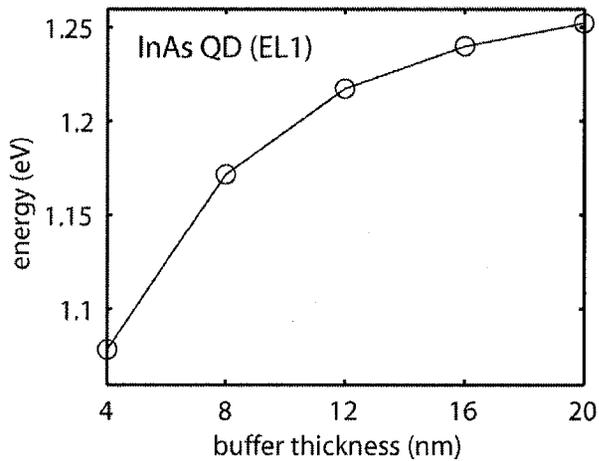
Disorder depends on buffer size !



Outline

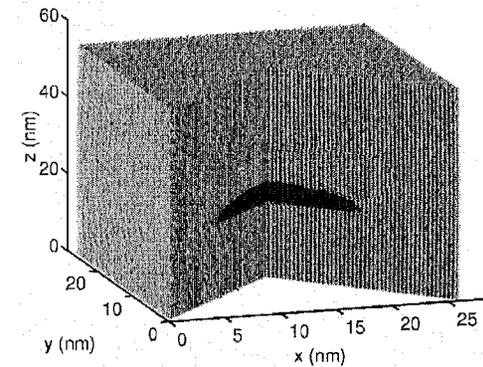
- **Motivation.**
- **High Performance Computing .**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Ground State Energy Dependence on Buffer Size

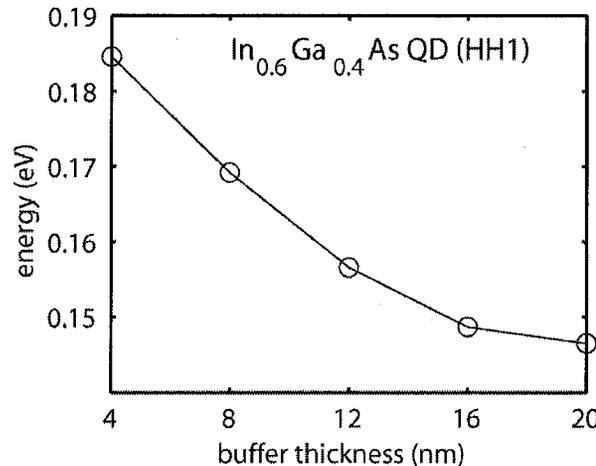
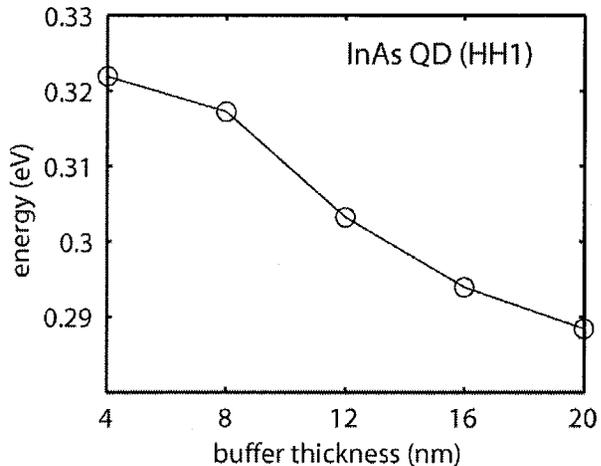
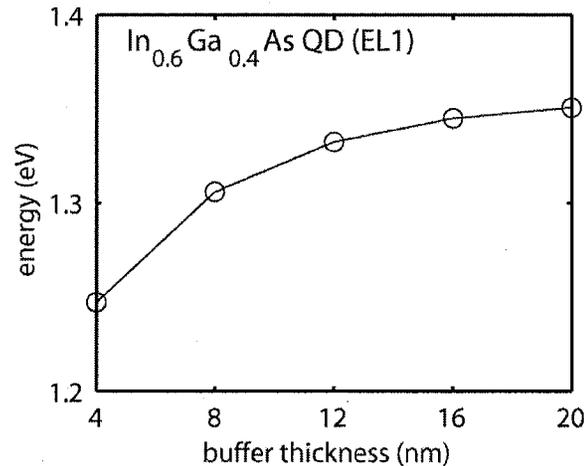
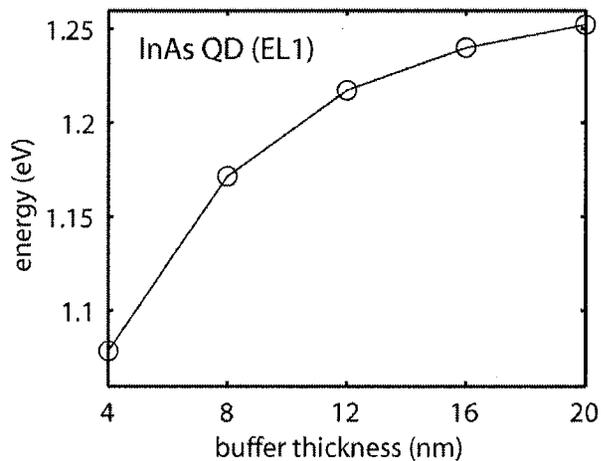


- Quantum dot:
30nm diameter
5nm height

- Vary GaAs buffer
from 4nm to 20nm
in all directions

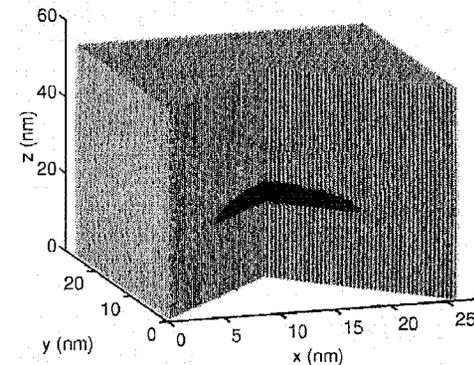


Ground State Energy Dependence on Buffer Size

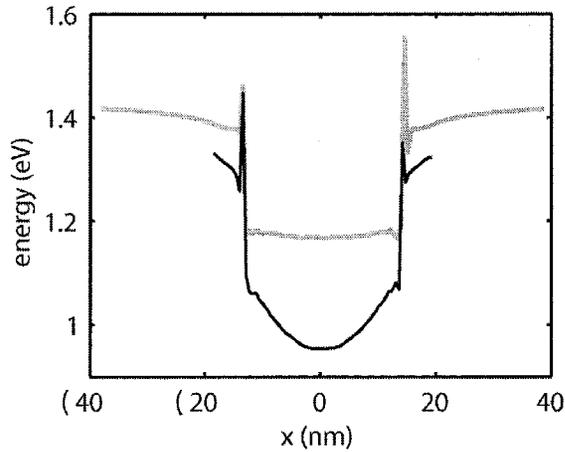


- Quantum dot: 30nm diameter 5nm height

- Vary GaAs buffer from 4nm to 20nm in all directions

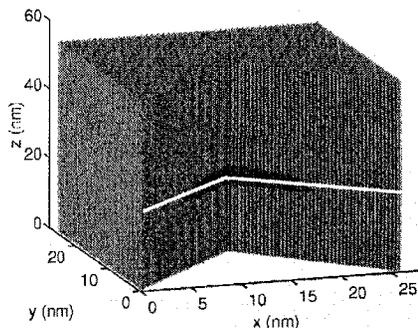


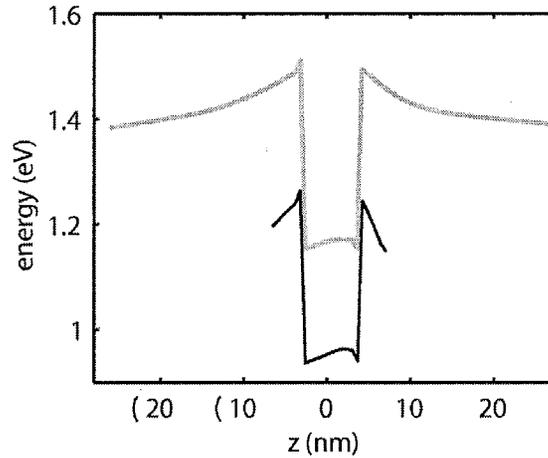
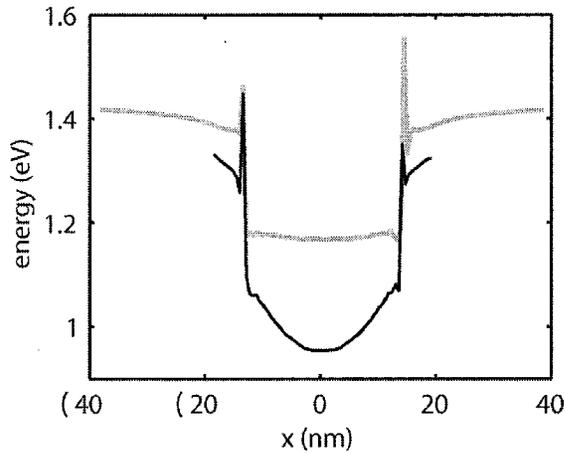
- Electron and hole ground states depend strongly on the GaAs buffer size
- Dependence is weaker for the electron states in the alloyed dot.



Strain Effects on Local Band Structure

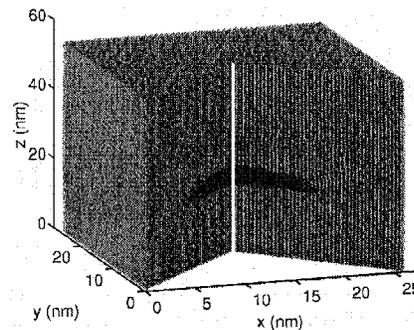
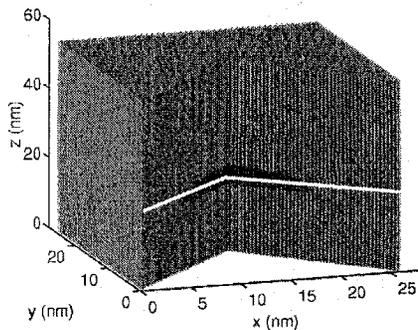
- Strain shows a long-range effect
- Electron confinement in x changes shape



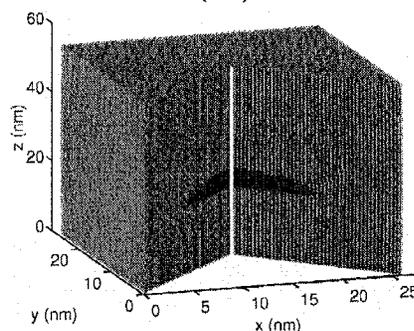
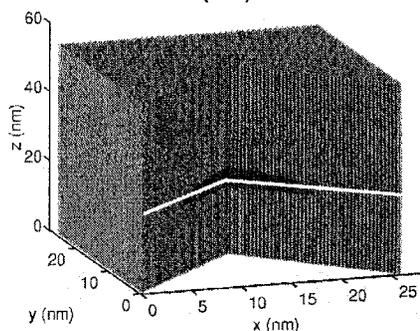
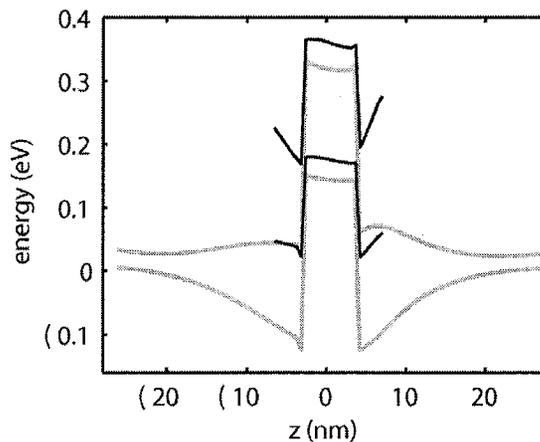
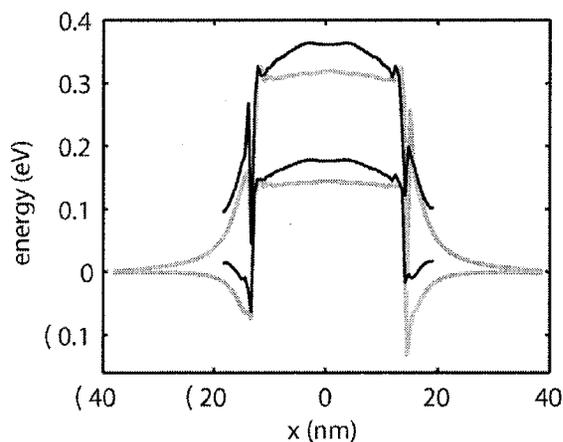
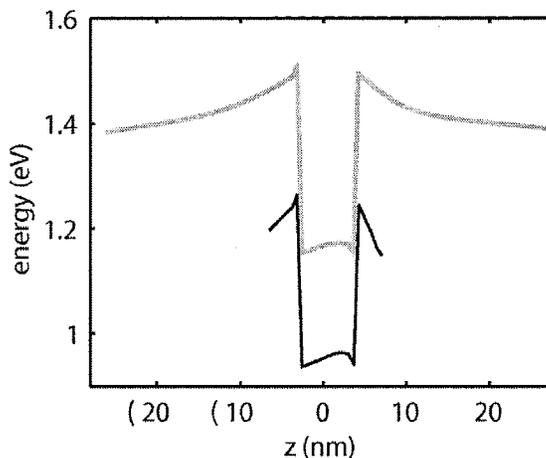
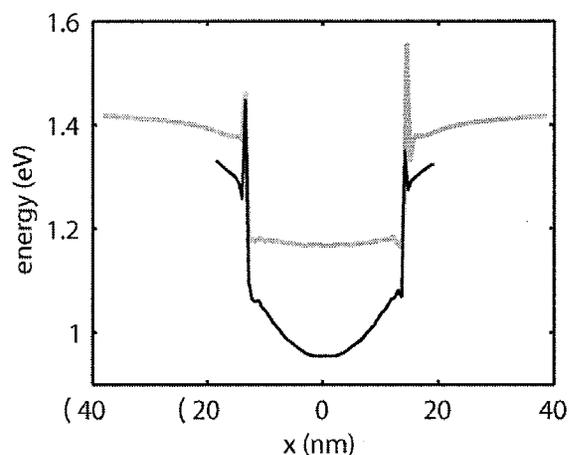


Strain Effects on Local Band Structure

- Strain shows a long-range effect
- Electron confinement in x changes shape
- Electron confinement in z shows vertical shift

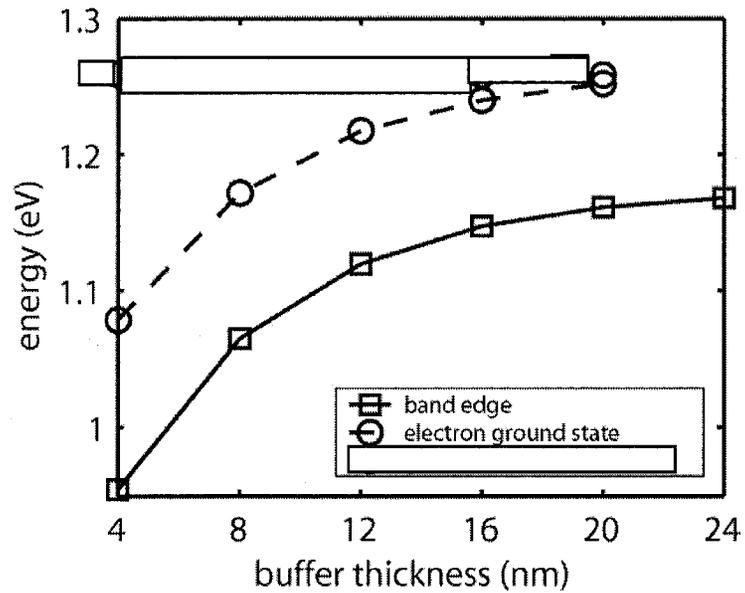


Strain Effects on Local Band Structure



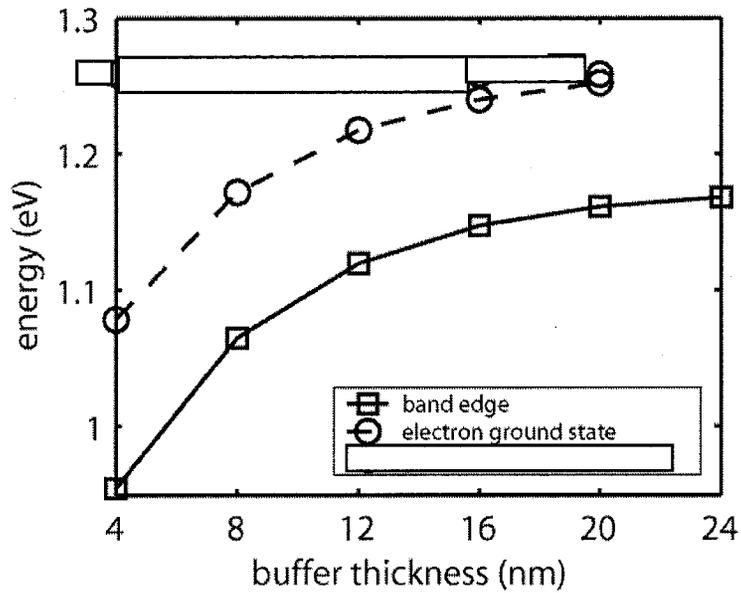
- Strain shows a long-range effect
- Electron confinement in x changes shape
- Electron confinement in z shows vertical shift
- Hole confinement in x small modulations
- Hole confinements in z vertical shift, no convergence yet!

Bandedges and Eigenstates

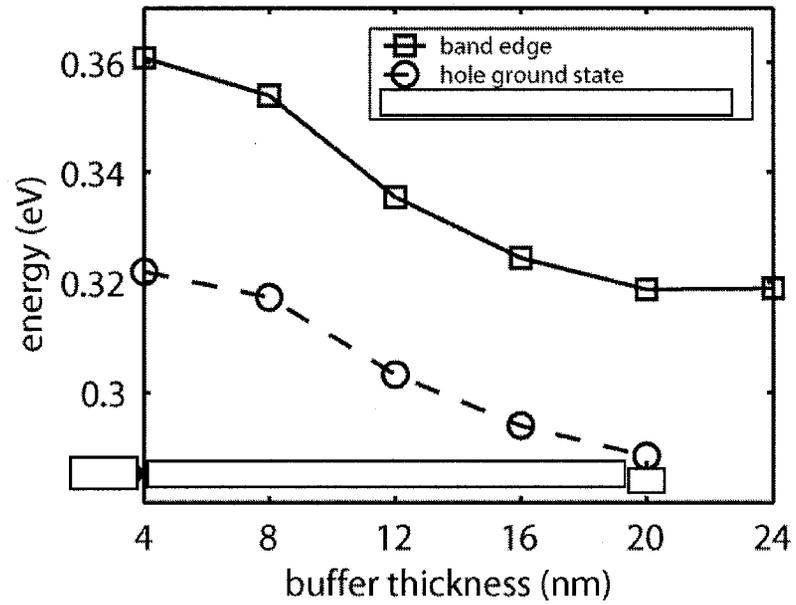


- **Electron ground state follows the bottom of the conduction band closely**

Bandedges and Eigenstates

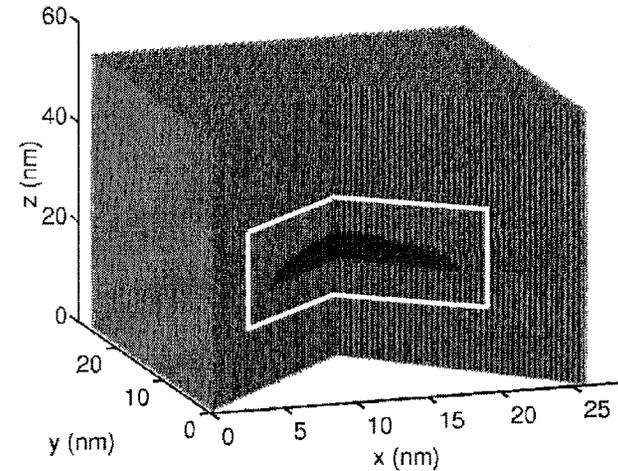
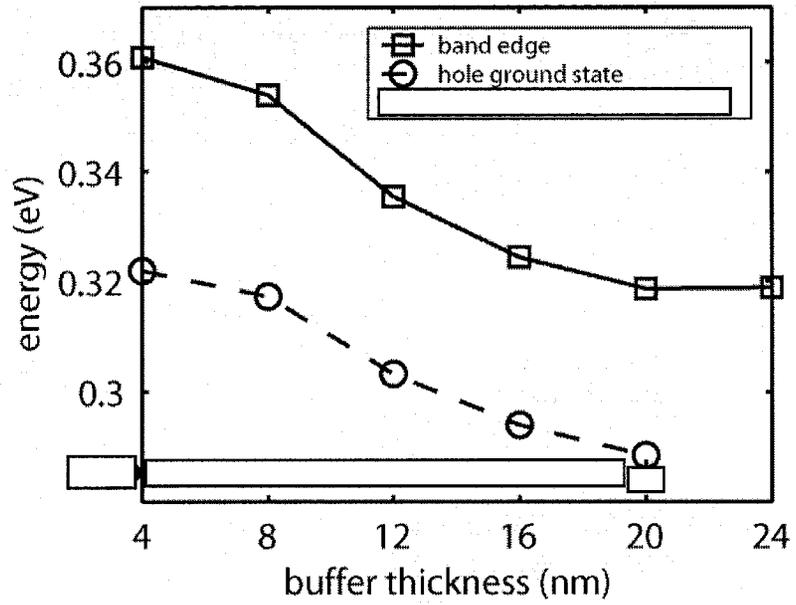
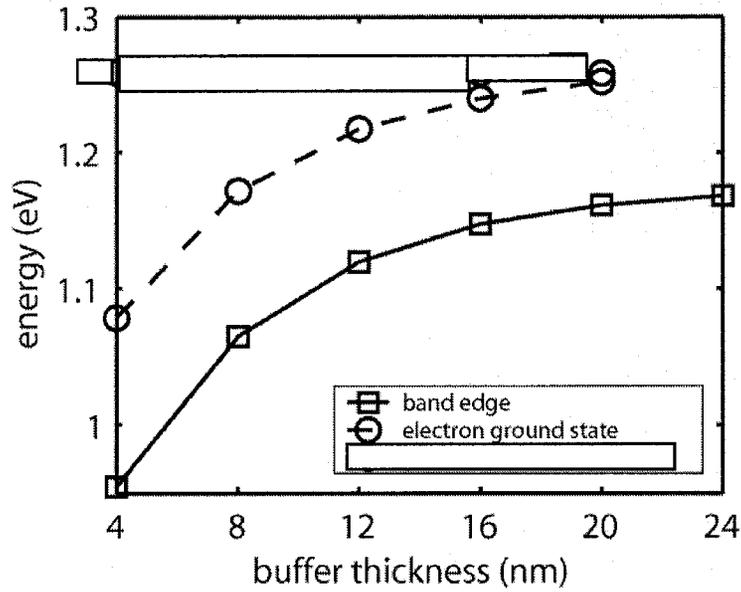


- **Electron ground state follows the bottom of the conduction band closely**

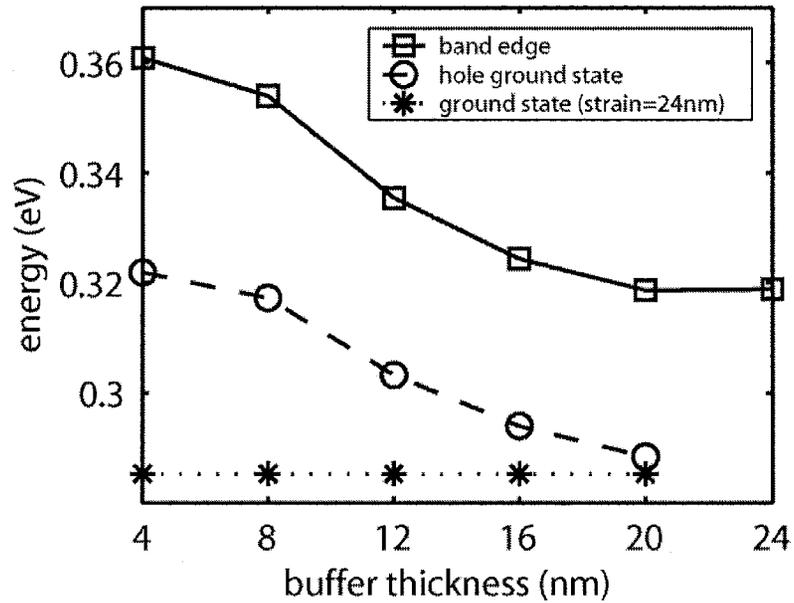
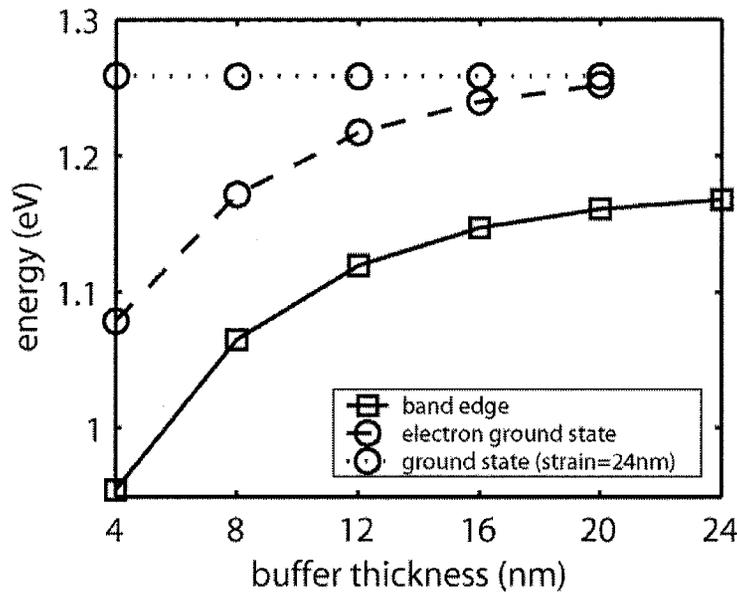


- **Valence ground state follows the top of the valence band closely**

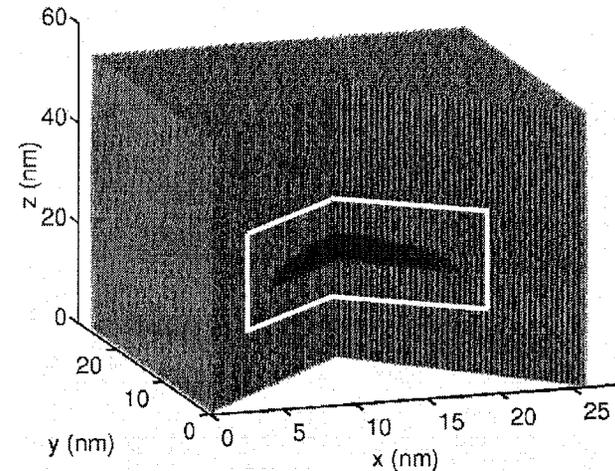
Decoupled Strain and Electronic Boundary Conditions



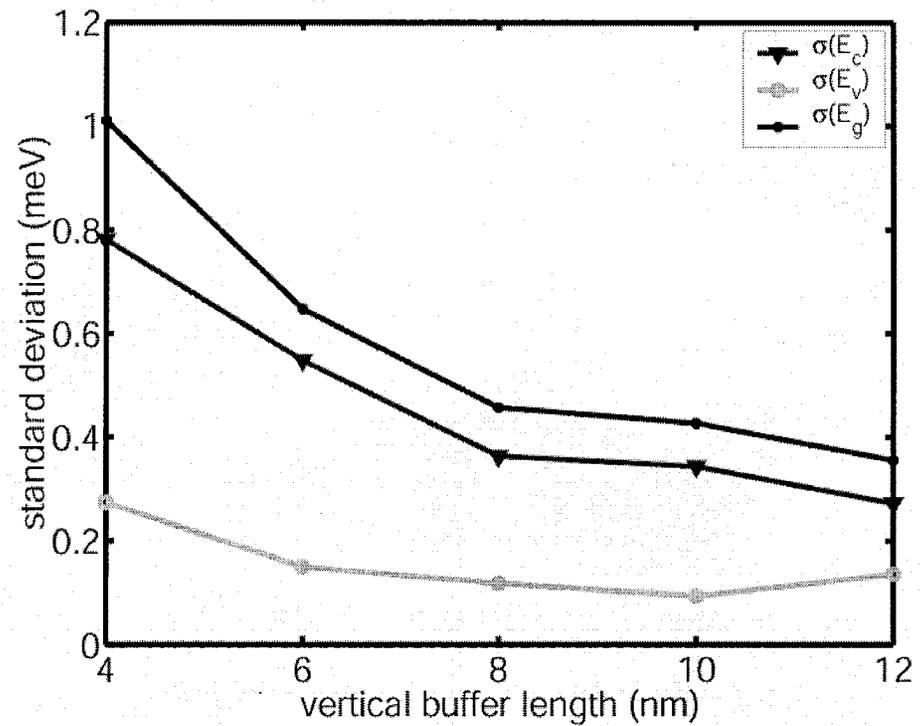
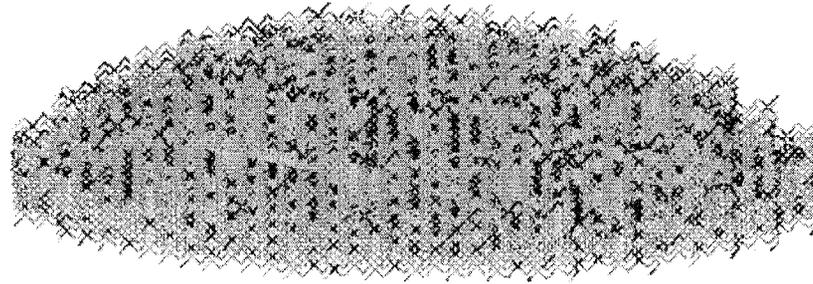
Decoupled Strain and Electronic Boundary Conditions



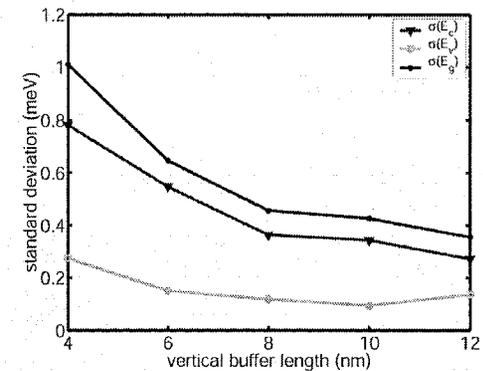
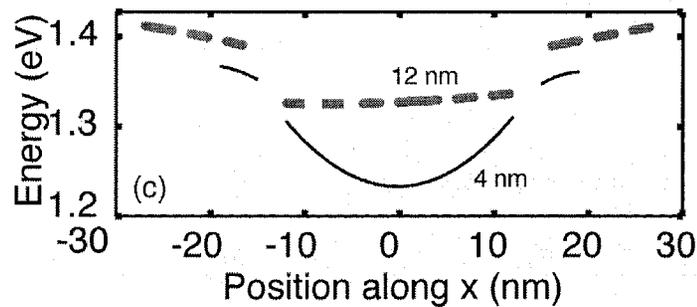
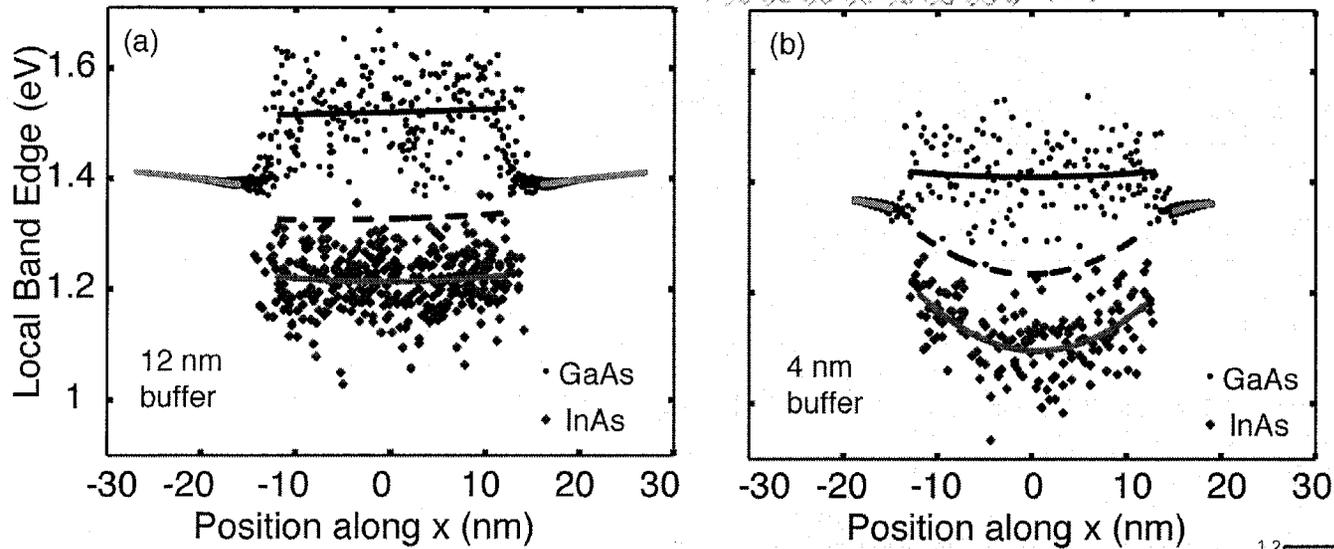
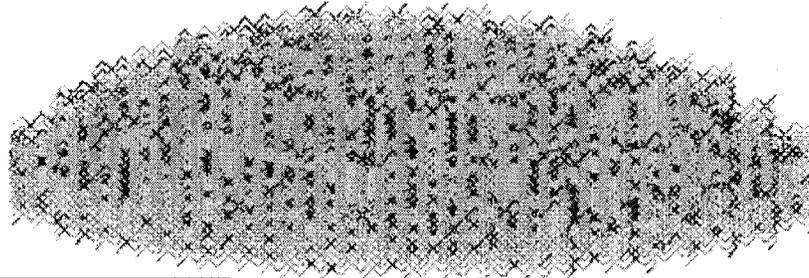
- Compute strain in 24nm buffer system (9 million atoms)
- Vary size of the electronic system buffer => Electronic states virtually unaffected
- Long-range strain effects dominate the quantum dot states.
- Neighboring dots will have strong effects!
- Hard-wall electronic boundary conditions have little effects.



Local Alloy Bandstructure for Different Buffers



Local Alloy Bandstructure for Different Buffers



Outline

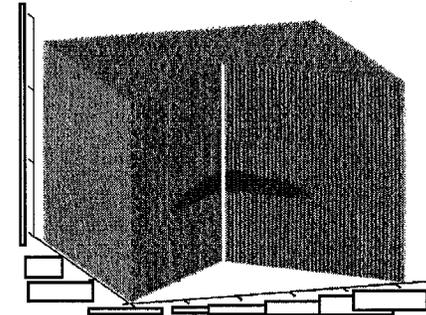
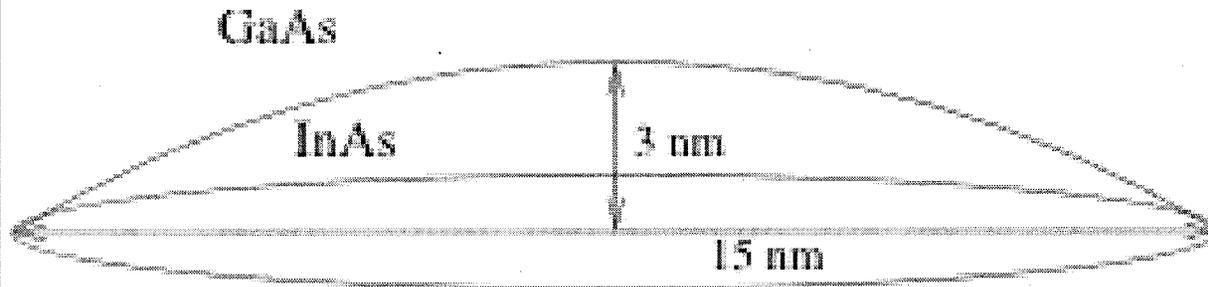
- **Motivation.**
- **High Performance Computing .**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Outline

- **Motivation.**
- **High Performance Computing .**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Magnetic-Field Effects in InAs Dot

- **System geometry**



- **Strain profile model:** Atomic elasticity model

[P. N. Keating, Phys. Rev. B **145**, 637 (1966)]

Strain energy as a function of bond length and bond angle.

GaAs strained buffer is 15nm in all directions (total of 2,764,600 atoms)

- **Electronic structure model:** Tight-binding Hamiltonian

Basis orbitals: $sp^3d^5 s^*$, parameters generated by a genetic algorithm.

Matrix Size : 2,090,880 = 104,544 atoms X 10 basis orbitals X 2 spins

- **Eigenvalue solver:** Arnoldi method with PARPACK

Computation on a Beowulf cluster with 30 nodes.

Currently memory limited, in process of system upgrade right now.

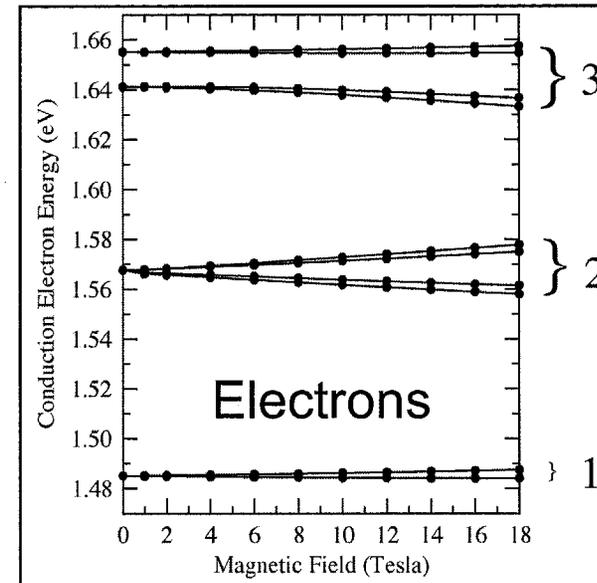
Magnetic-Field Effects on Confined States

- Study InAs/GaAs QDs
- Zeeman Interaction splits the levels into spin-up and -down levels.
- Effective g-factor ($g^* = (E_{\uparrow} - E_{\downarrow}) / \mu_B B$)

Electrons:

- g^* ranges from 2 to 3.5.
- InAs dot g^* is very different from g^* of InAs bulk (-15).
- Experimental measurements report $g^* = 0.5 - 1.6$ for InAs dots.

[Thornton et al., Appl. Phys. Lett. **73**, 354 (1999)]



Magnetic-Field Effects on Confined States

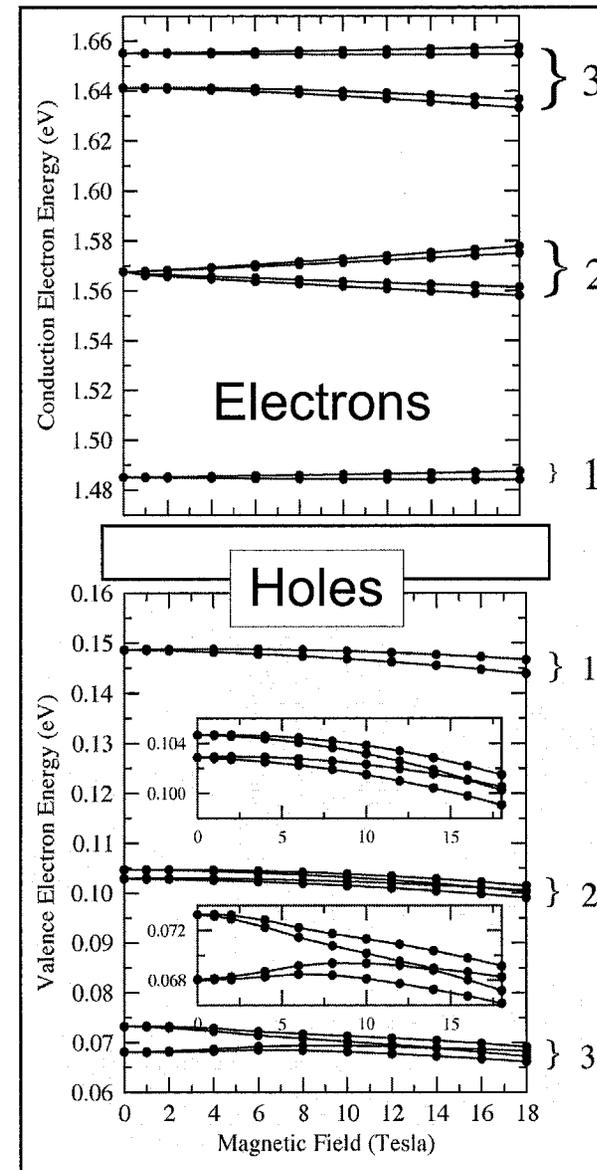
- Study InAs/GaAs QDs
- Zeeman Interaction splits the levels into spin-up and -down levels.
- Effective g-factor ($g^* = (E_{\uparrow} - E_{\downarrow}) / \mu_B B$)

Electrons:

- g^* ranges from 2 to 3.5.
 - InAs dot g^* is very different from g^* of InAs bulk (-15).
 - Experimental measurements report $g^*=0.5-1.6$ for InAs dots.
- [Thornton et al., Appl. Phys. Lett. **73**, 354 (1999)]

Holes:

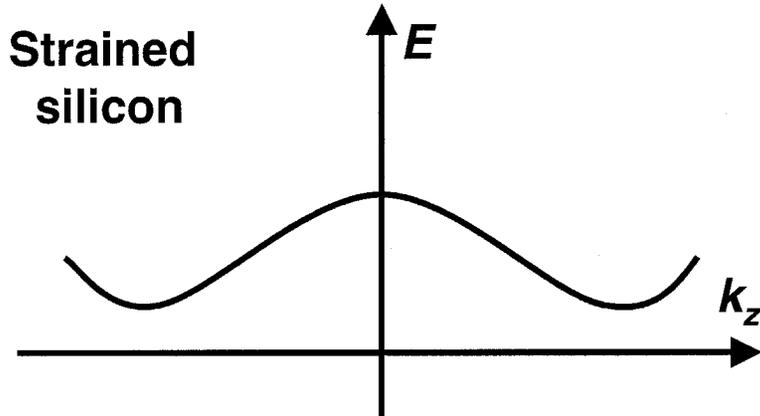
- Zeeman interaction splits hole levels into $J_z = 3/2$ and $-3/2$ levels.
- Zeeman interaction couples closely-spaced hole levels.
- g^* varies from 0.65 to 2.66



Outline

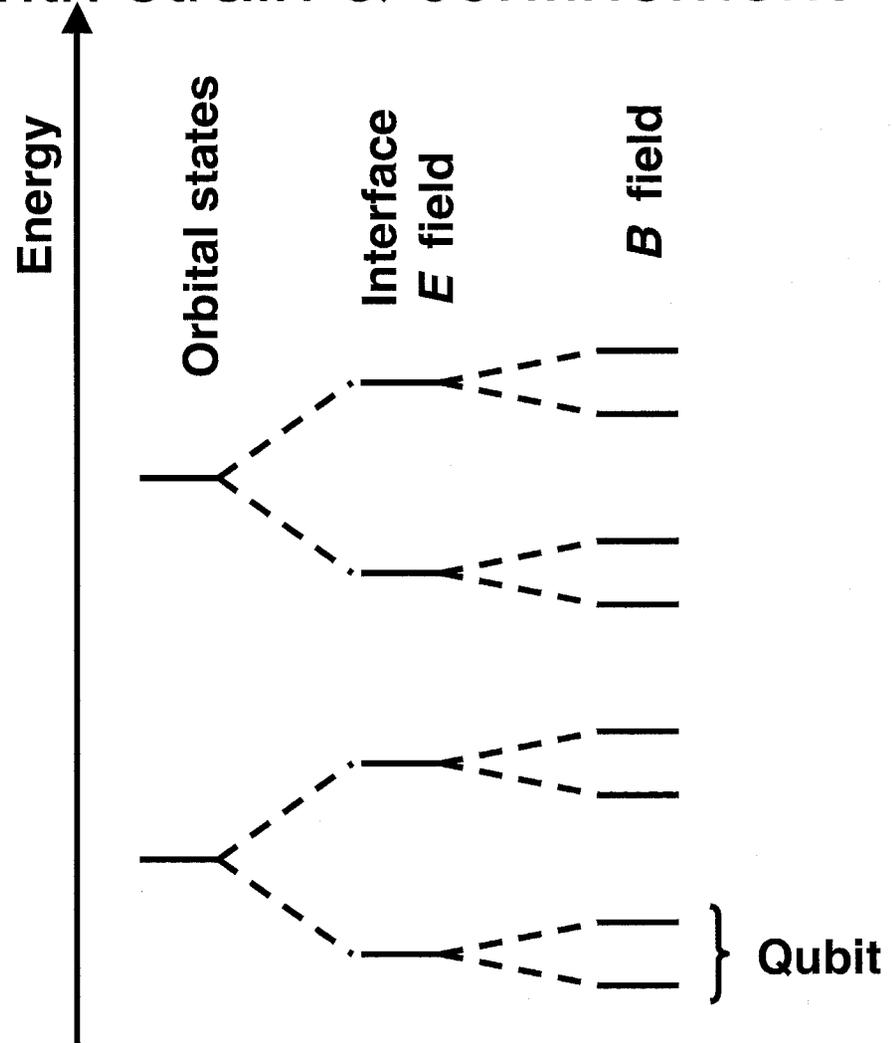
- **Motivation.**
- **High Performance Computing .**
- **Alloy Disorder in InGaAs Quantum Dots (~1 Million Atoms).**
- **Long-Range Strain in InGaAs Quantum Dots (~20 Million Atoms).**
- **Magnetic Fields in InAs Quantum Dots.**
- **Quantum Computing in Si?
Lifting of the valley degeneracies.**
- **Conclusions**

Quantum Dot Quantum Computing in Si: Lifting Degeneracies with strain & confinement

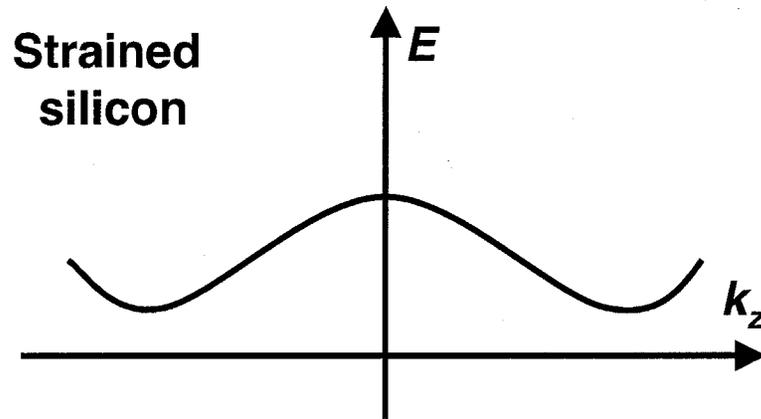


Valley degeneracy in X direction is broken by interface and electric field

Are the qubit states separated enough from higher energy states?

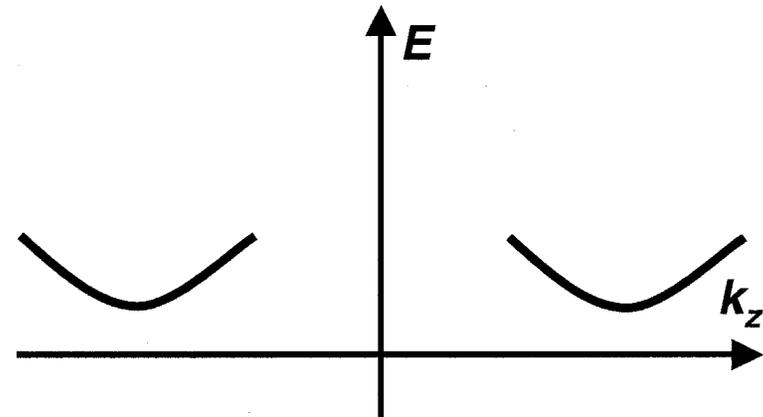


Quantum Dot Quantum Computing in Si: Lifting Degeneracies with strain & confinement



Valley degeneracy in X direction is broken by interface and electric field

Atomistic approach deliver these details automatically.



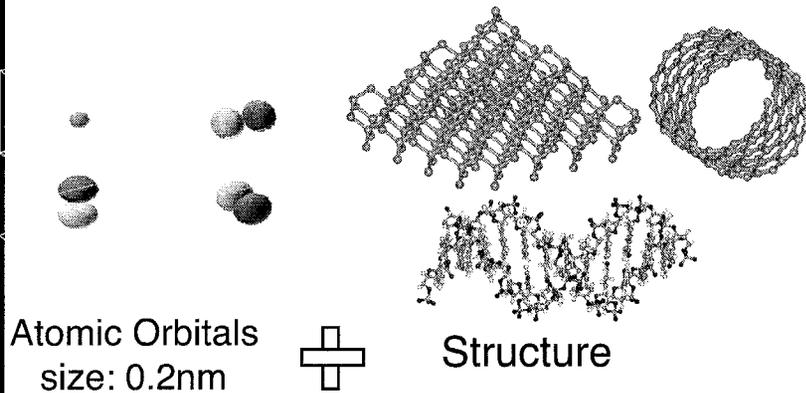
Standard Approach:

Effective Mass

Single, parabolic band

Need high-powered physics, (hand-waiving) coupling constant to couple the valleys.

Mapping of Orbitals to Bulk Bandstructure

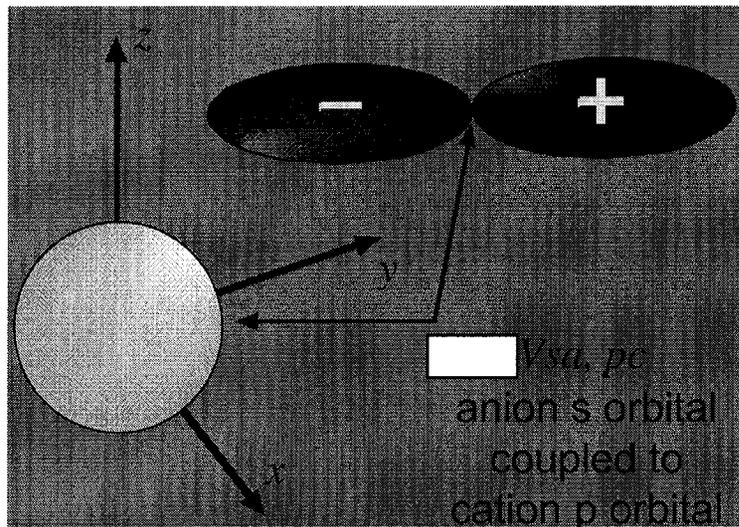


Bulk Semiconductors are described by:

- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

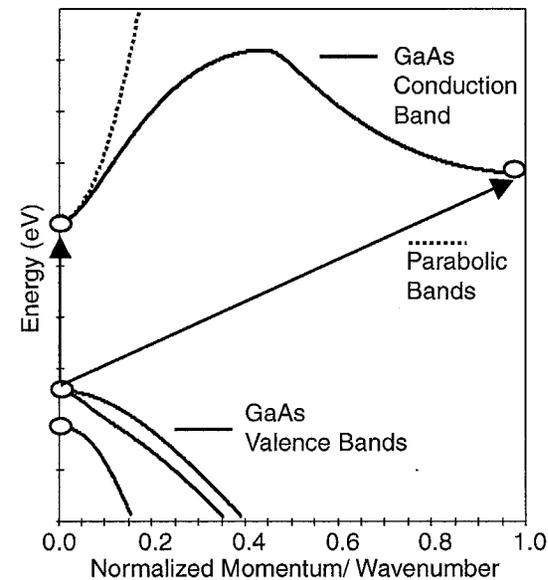
Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters



High Dimensional Fitting Problem

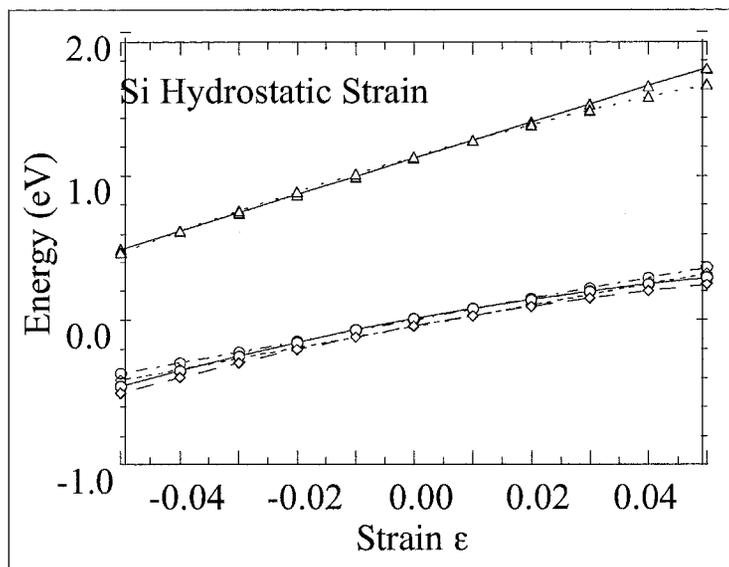
Numerical and analytical approach developed



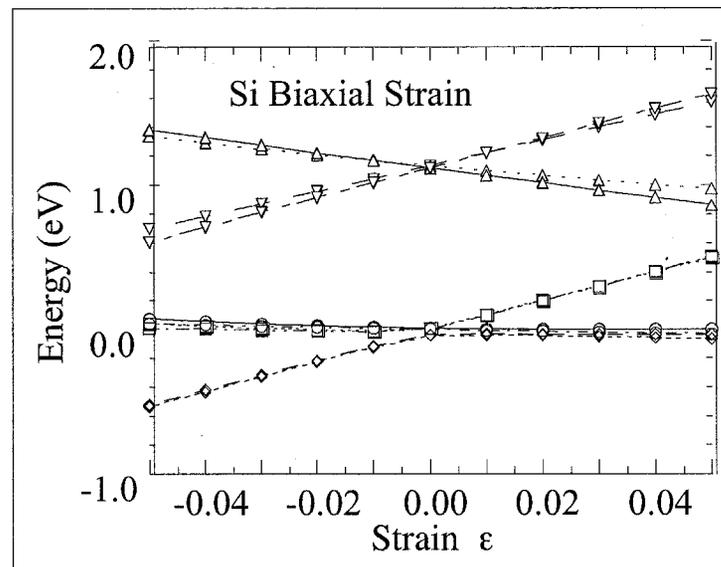
15-30 theoretical interaction energies

10-30 data points of bands and masses

Bulk Si: Strain Behavior

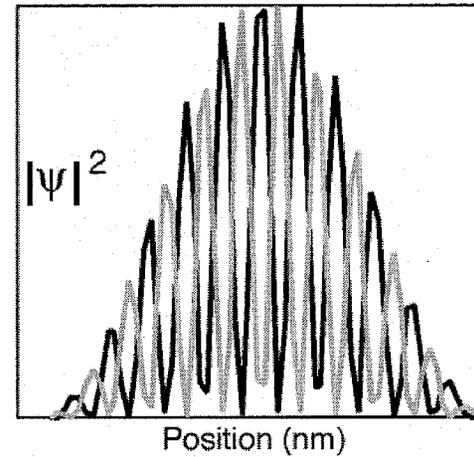
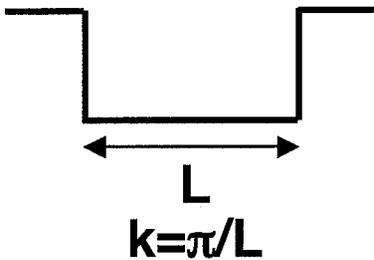
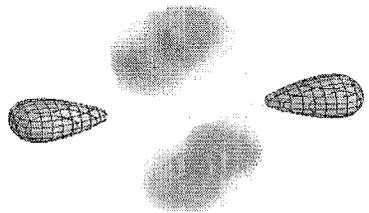


**Hydrostatic distortions:
match k.p theory and experiment**

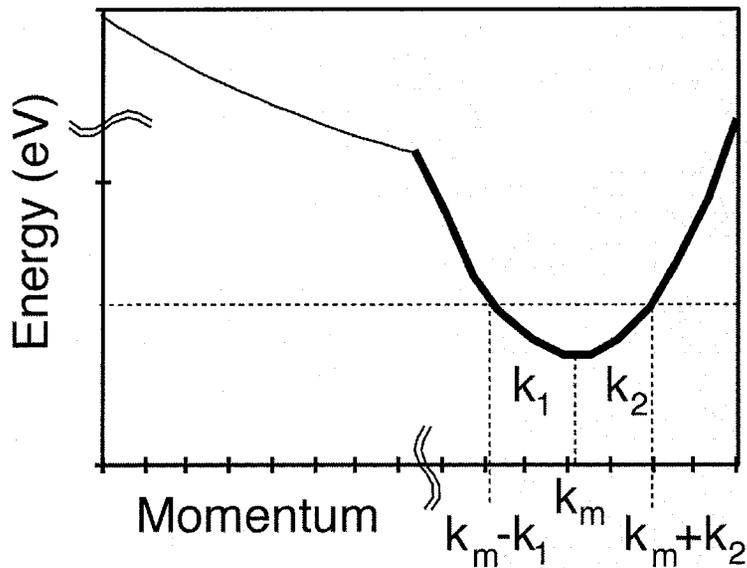


**Bi-Axial distortions:
match k.p theory and experiment**

1D Confinement Creates Valley Splitting:



Valley Splitting $\Delta E \sim 1 \text{ meV}$



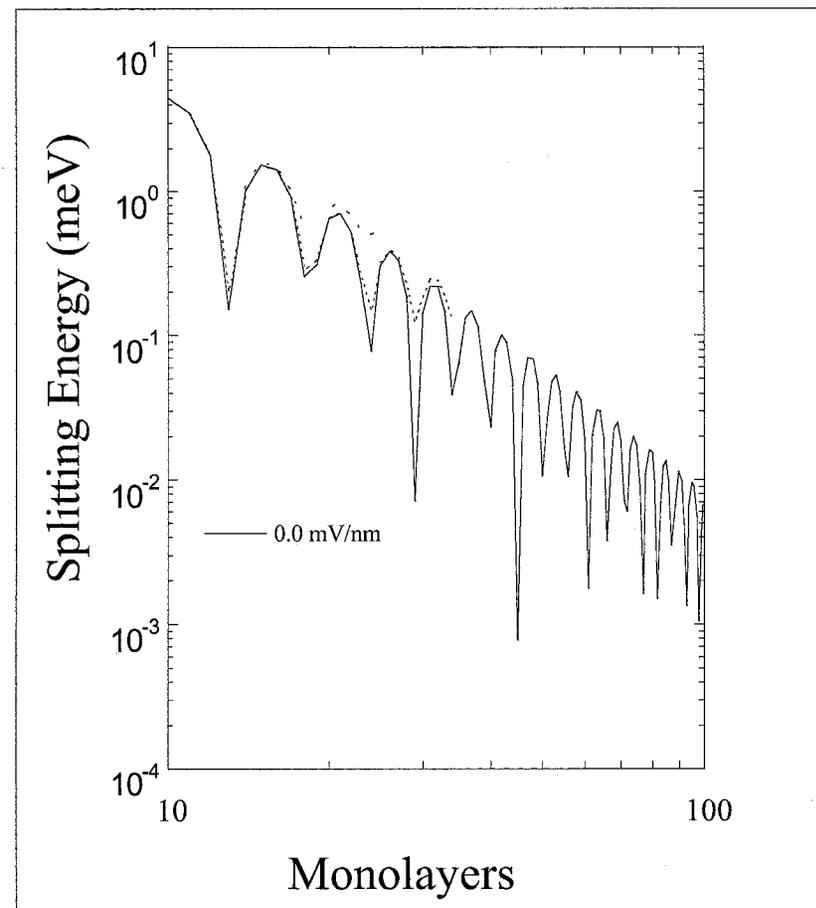
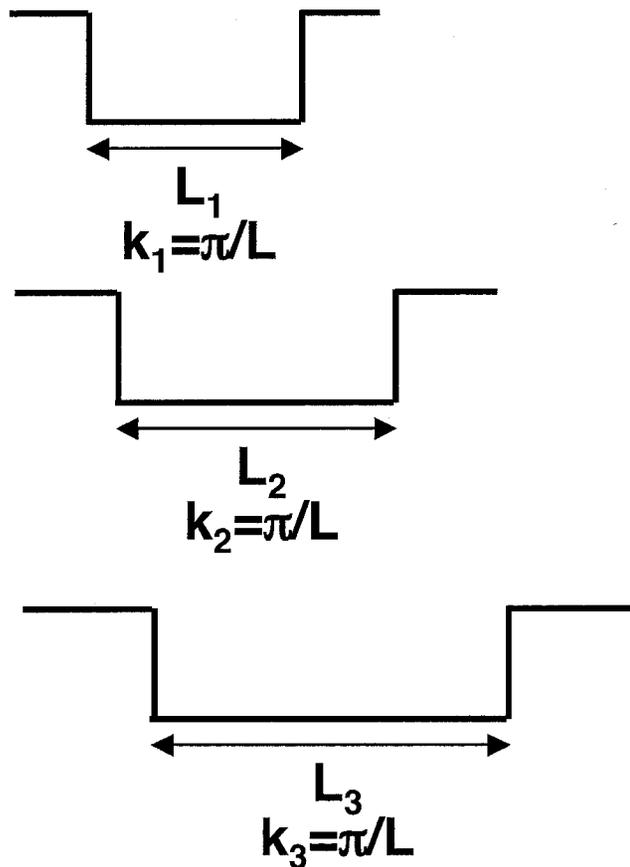
4 propagating states



2 bound states
 $k_{1,2}$ envelope
 k_m fast oscillations

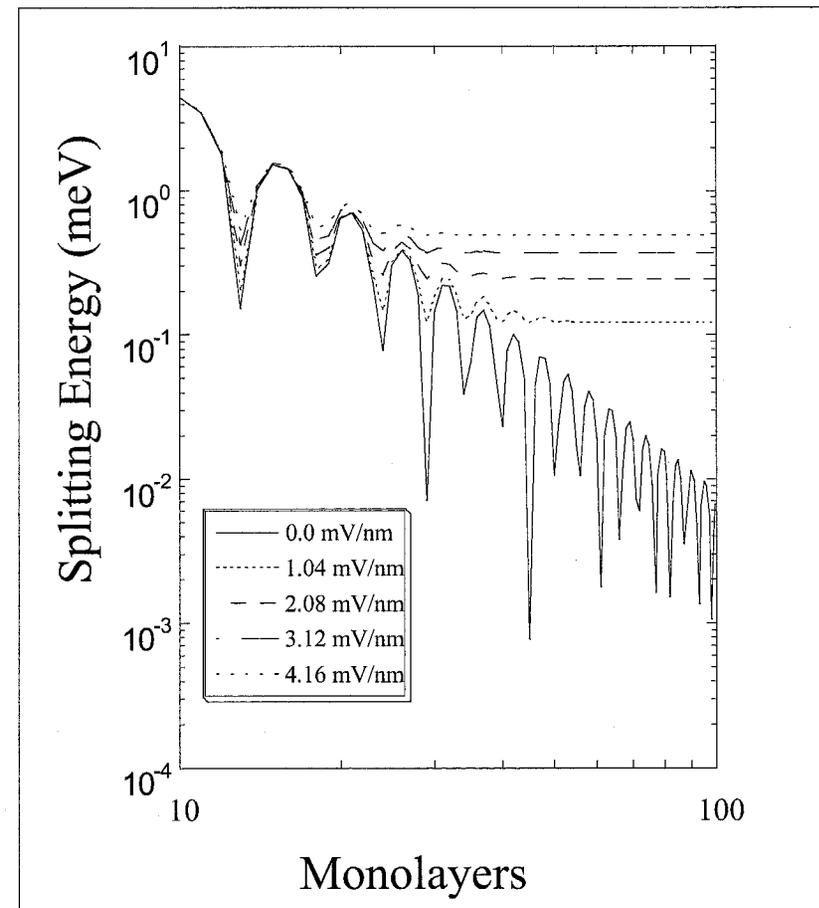
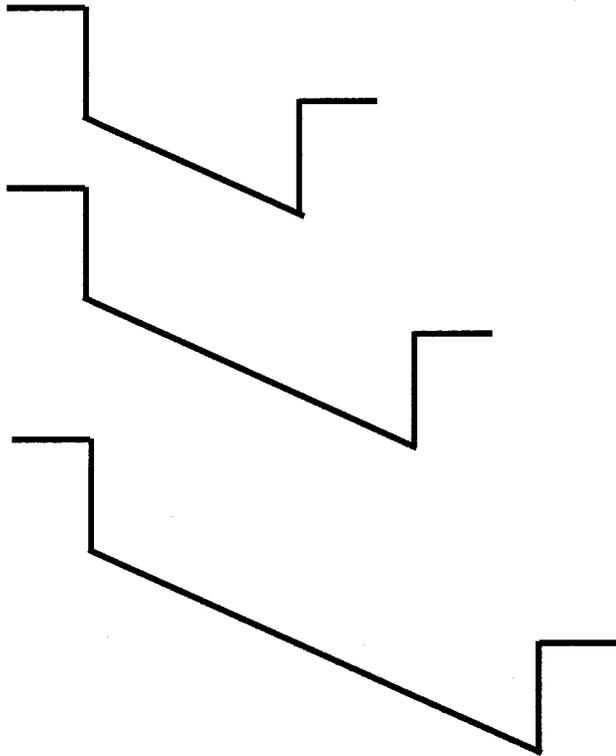
Splitting Behavior With Quantum Well Width

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers (decay as ML^{-3})



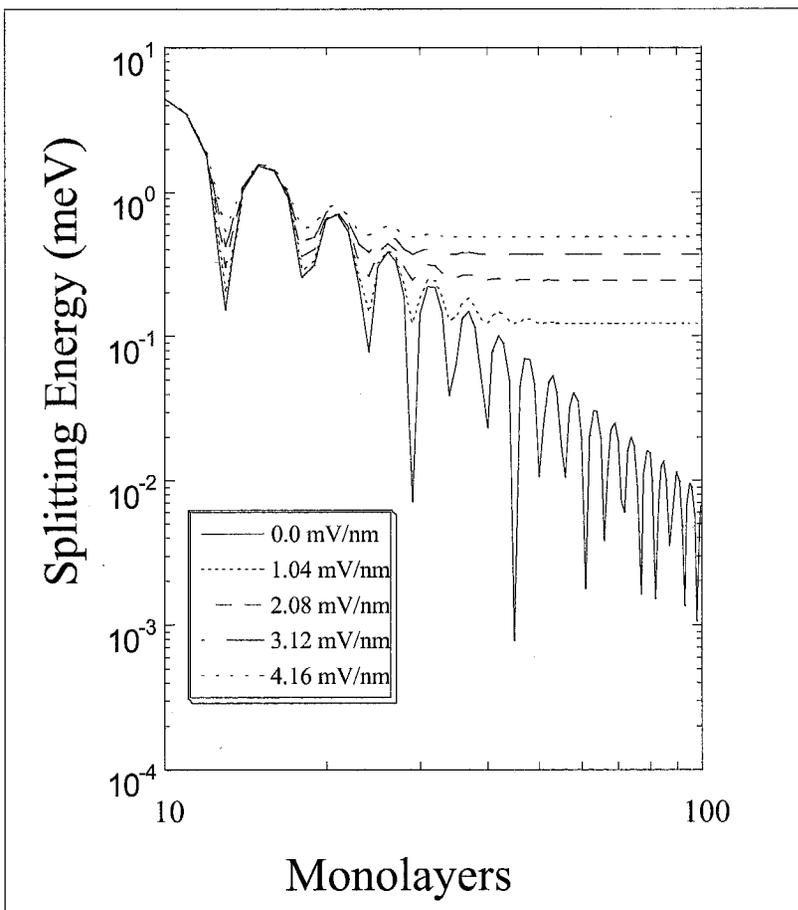
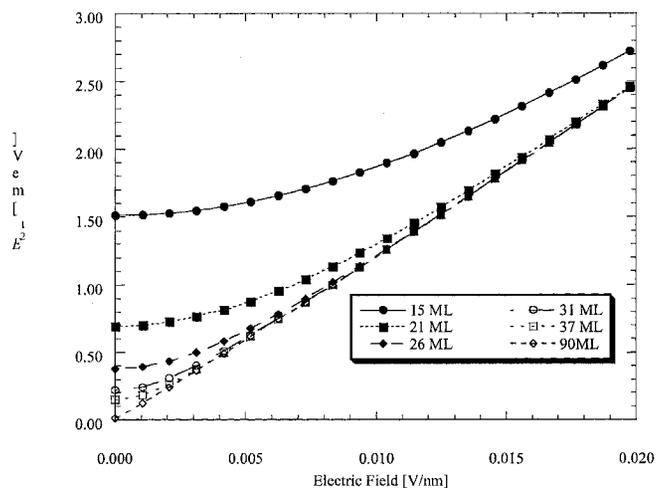
Splitting Behavior With Quantum Well Width and Electric Field

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting



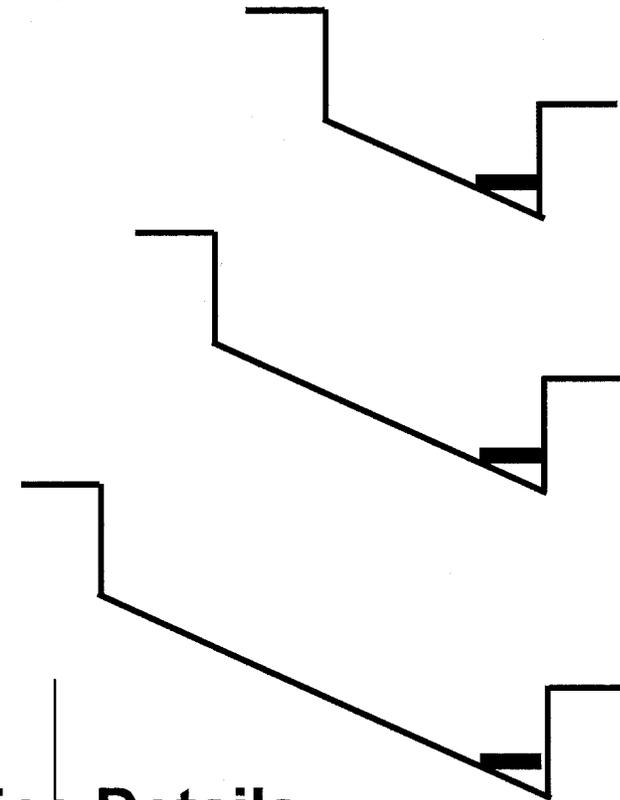
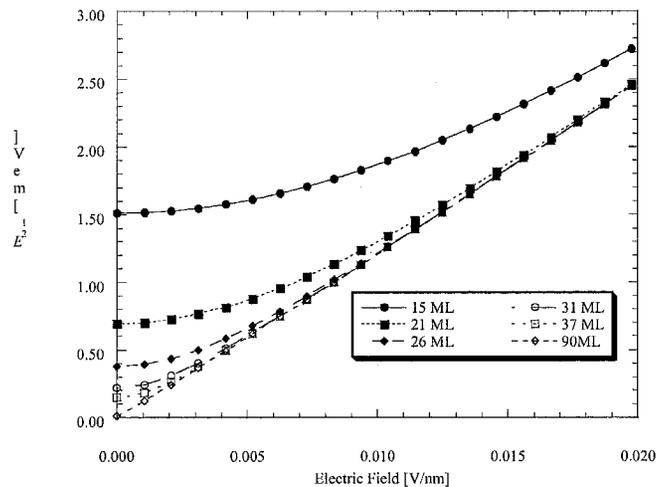
Splitting Behavior With Quantum Well Width and Electric Field

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
- For fixed L , splitting linear at high field, nonlinear at low field



Splitting Behavior With Quantum Well Width and Electric Field

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
- For fixed L , splitting linear at high field, nonlinear at low field



**Device Details
(structure, materials,
local fields,)
determine energy splitting**

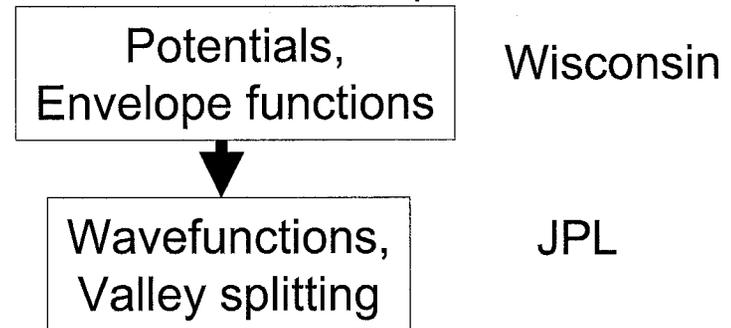
Hybrid Approach to Valley Splitting in 3D Qubits

Problem:

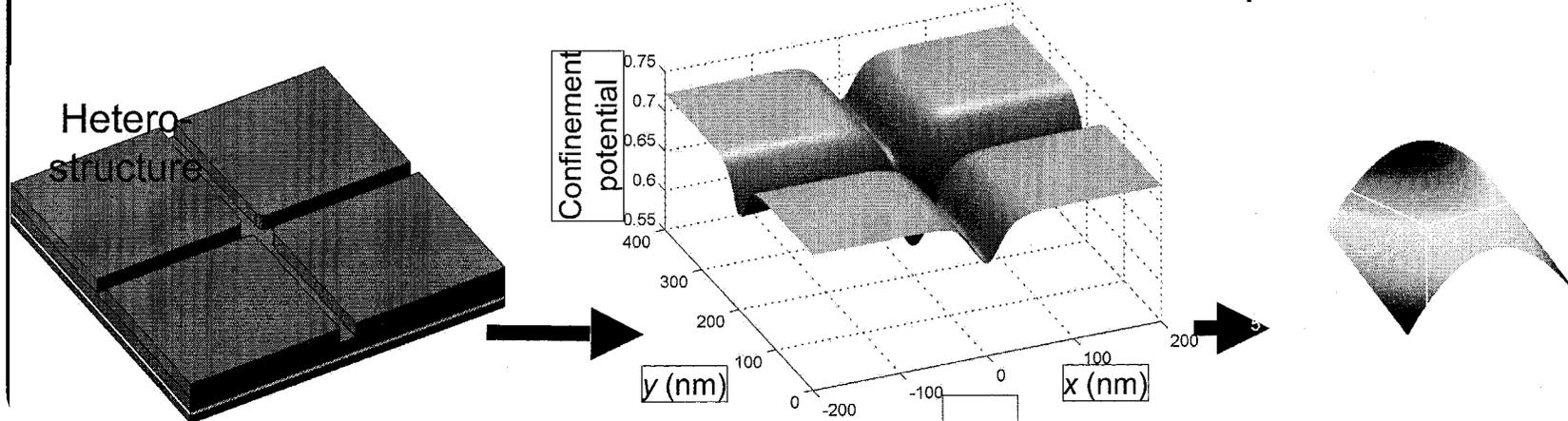
- Valley splitting is strongly affected by local, inhomogeneous E fields that are not necessarily parallel to z .
- ⇒ Requires 3D treatment.
- Atomistic approach, including gates and heterostructure, is too large for NEMO3D alone.
- ⇒ Hybrid mesoscopic/atomistic simulations.

Approach:

- Electrostatic potentials, including gate and image potentials, self-consistency, are computed at Wisconsin for heterostructures with envelope functions.



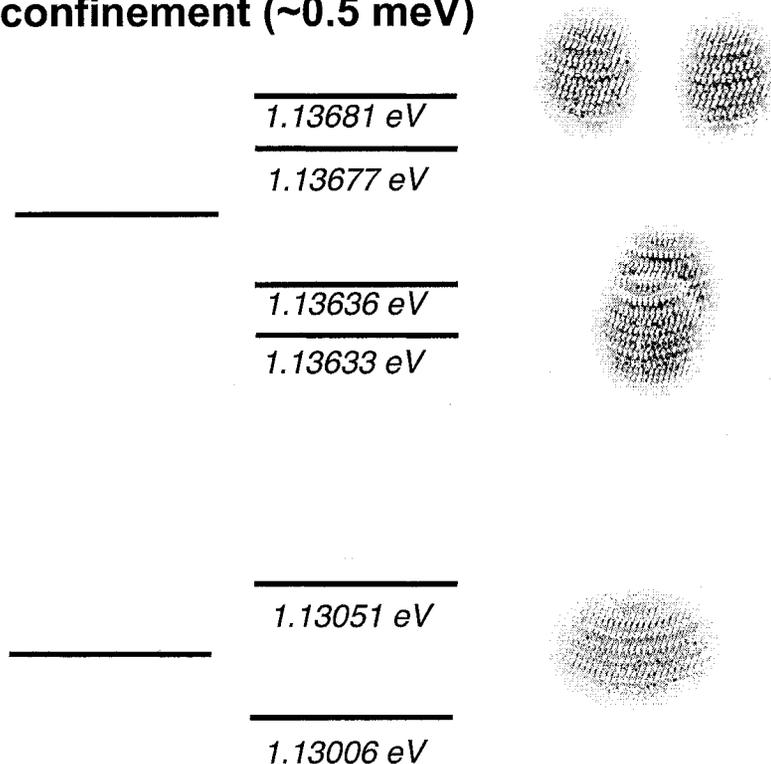
- NEMO3D computes exact wavefunctions in quantum dot.



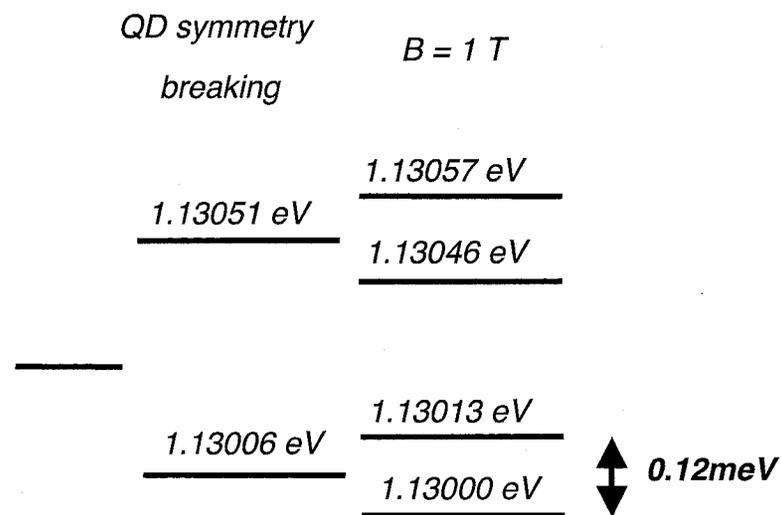
Relative Size of State Splitting

3-D Electronic structure of low-lying states

- Valley splitting due to breaking of translational invariance is typically smaller than splitting due to confinement (~ 0.5 meV)



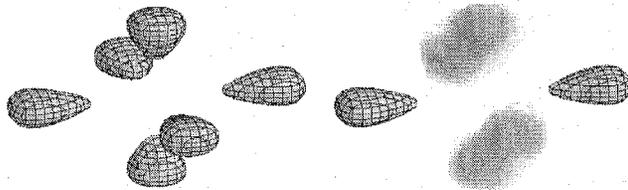
- Even with a large $B=1.0$ T, Zeeman splitting is much smaller than valley splitting (~ 0.12 meV).



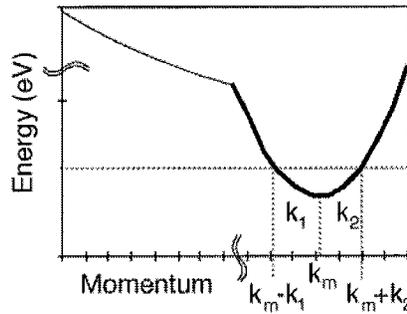
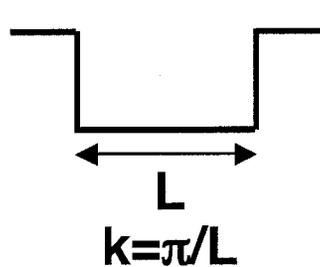
Quantum Dot Quantum Computing in Si:

Lifting Degeneracies - strain & confinement

- Bi-axial strain on Si. Lifting 4 of the 6 degenerate valleys $\Delta E > 100 \text{ meV}$



- Confinement in 1D: Valley Splitting $\Delta E \sim 1 \text{ meV}$



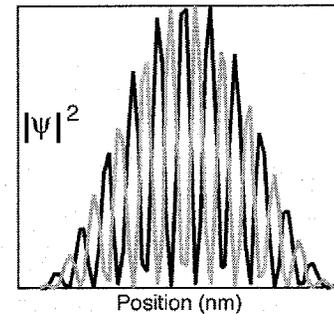
4 propagating states



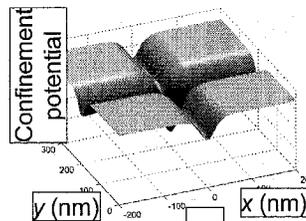
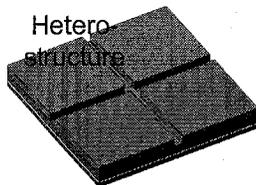
2 bound states

$k_{1/2}$ envelope

k_m fast oscillations



- Confinement in 3D: (1D heterostr. & 2D lat gates & mag. field) $\Delta E \sim 0.1 \text{ meV}$

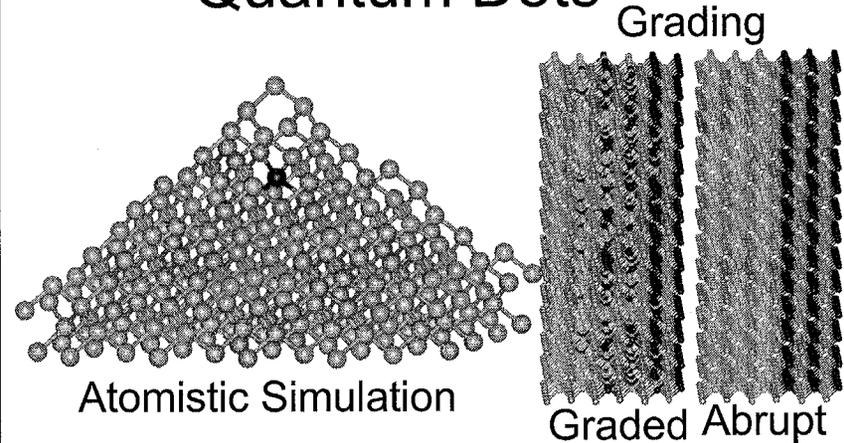


NEMO 3-D Conclusion / Future Vision

Atomistic Simulation (NEMO 3-D):

- Fitting tight binding sp^3s^* , $sp^3d^5s^*$
- General structure input
- Several million atom solutions
- Parallel eigenvalue solvers
- Strain simulations
- Studied effects of alloy disorder on optical transitions and wavefunctions.

Quantum Dots



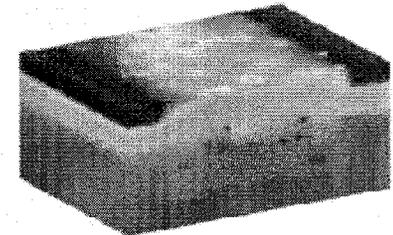
=> Quantum Computing

Extension of NEMO 3-D to Spintronics:

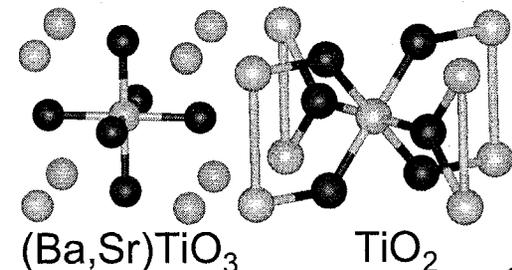
- Arbitrary magnetic fields
- Magnetic impurities
- Many-body interactions (electrons, phonons, photons)
- Open boundary conditions
- Extension of NEMO 1-D to Spintronics:
 - DC Spin transport RTD-like structures
 - Time dependent spin - transport

End of SIA Roadmap

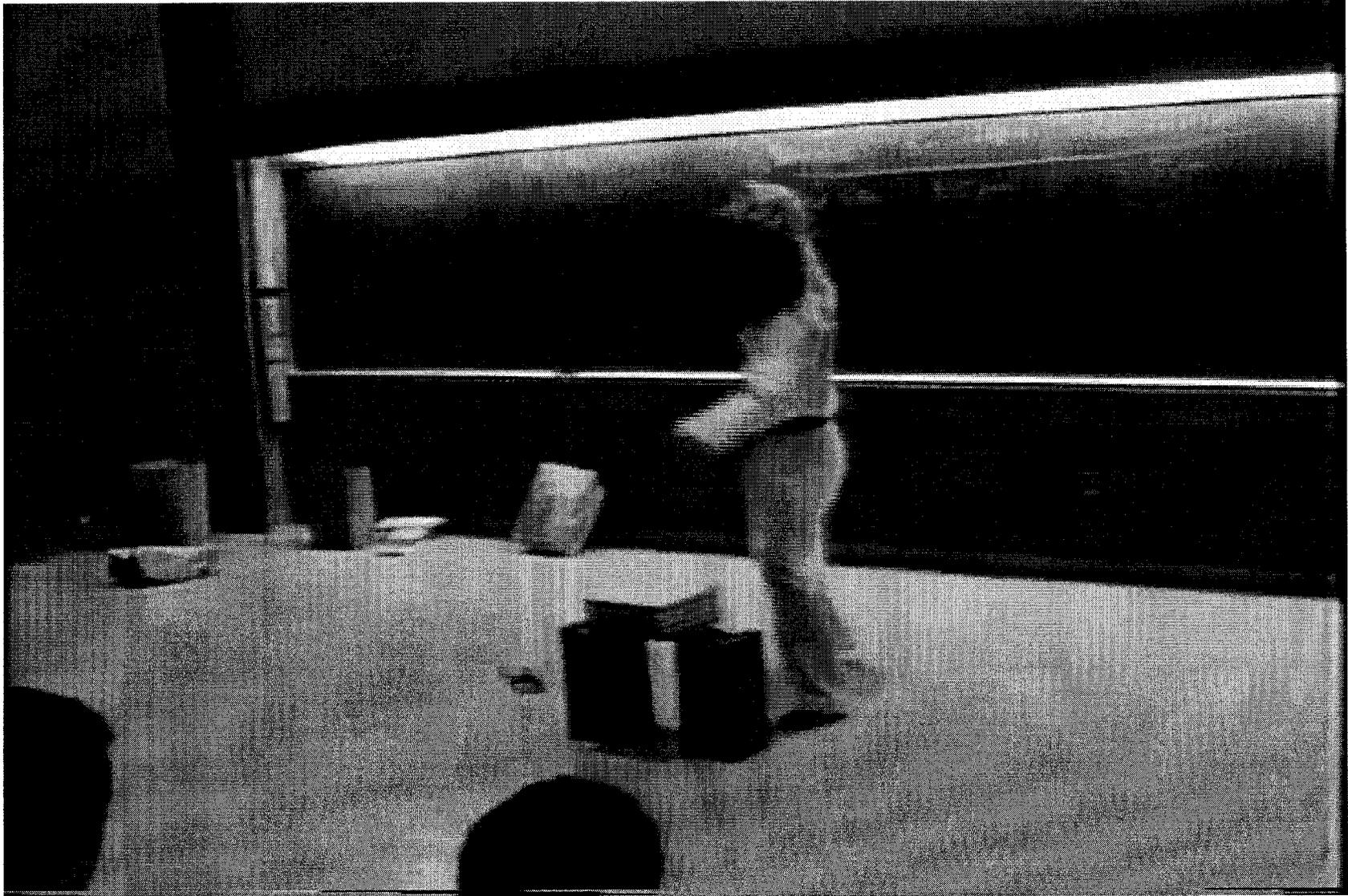
Dopant Fluctuations in Ultra-scaled CMOS



Electron Transport in Exotic Dielectrics



Questions? Breakthroughs?



JPL



Backup Slides

Inhomogeneous Broadening due to Alloy Disorder

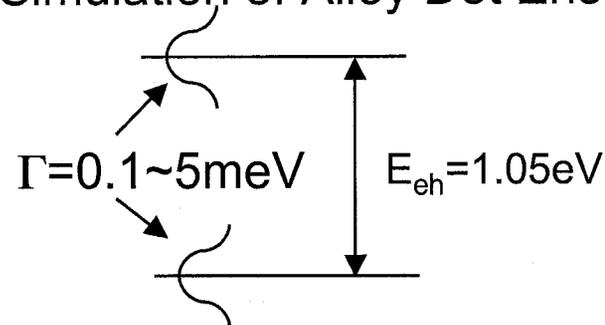
Problem:

- Cations are randomly distributed in alloy.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?
- Requires atomistic simulation tool.

Approach:

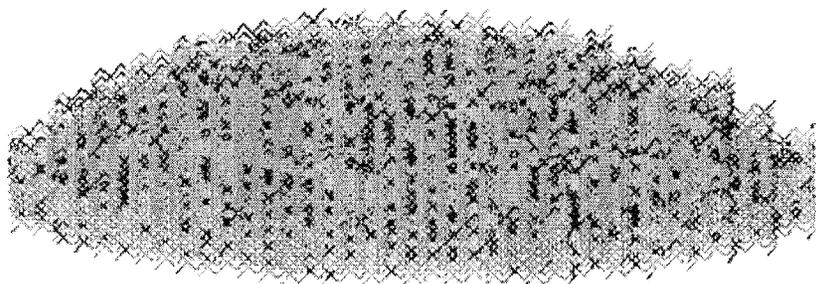
- Simulate a statistical ensemble of dots.
 - Identical in size and shape
 - Different only in cation ordering.

Simulation of Alloy Dot Ensemble



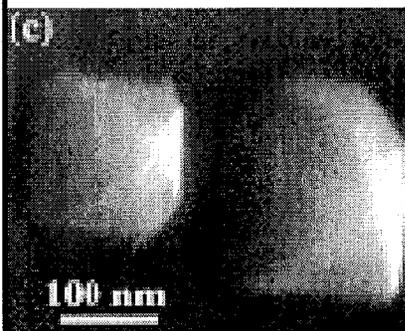
Measured $\Gamma = 34.6$ meV (R. Leon, PRB, 58, R4262)

1~5meV Represents Theoretical Lower Limit



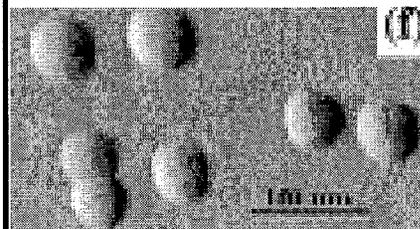
In_{0.6}Ga_{0.4}As Lens Shaped Dot

Diameter=30nm, Height=5nm, GaAs embedded
 ~1,000,000 Atom Simulation, sp³s* basis
 In and Ga atoms are randomly distributed
 Inhomogeneous Broadening?



**Quantum Dots:
 Self-assembled,
 InAs on GaAs.**

**Pyramidal or
 dome
 shaped**



**R. Leon et al,
 JPL (1998)**

Tight Binding Material Parameterization

Bulk Semiconductors are described by:

- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters

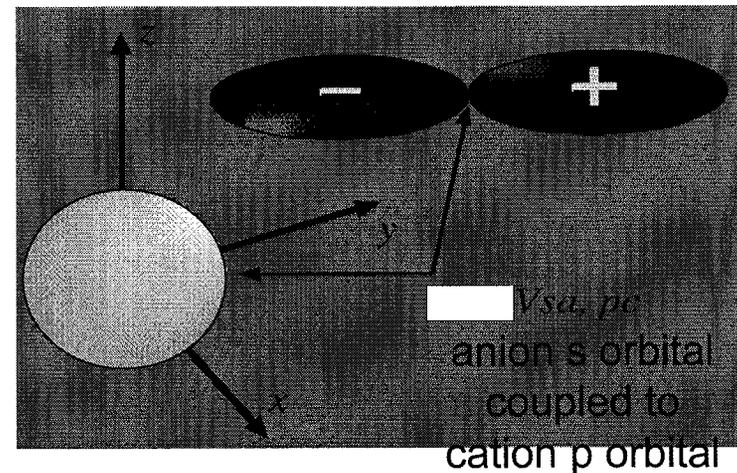
Analytical approach:

- Exact diagonalization at Γ for $sp^3d^5s^*$
- Formulas developed by Tim Boykin at UAH for effective masses and bandgaps from interaction energies

Numerical approach:

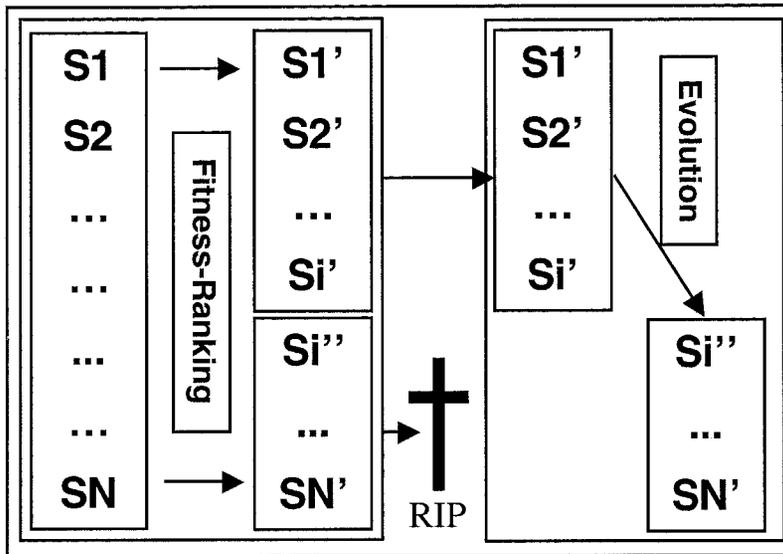
- Use a genetic algorithm to do fitting.

- Match experimental data in various electron transport areas of the Brillouin zone:
 - Effective masses of electrons at Γ , X and L
 - Effective masses of holes at Γ
 - Band edges at Γ , X and L



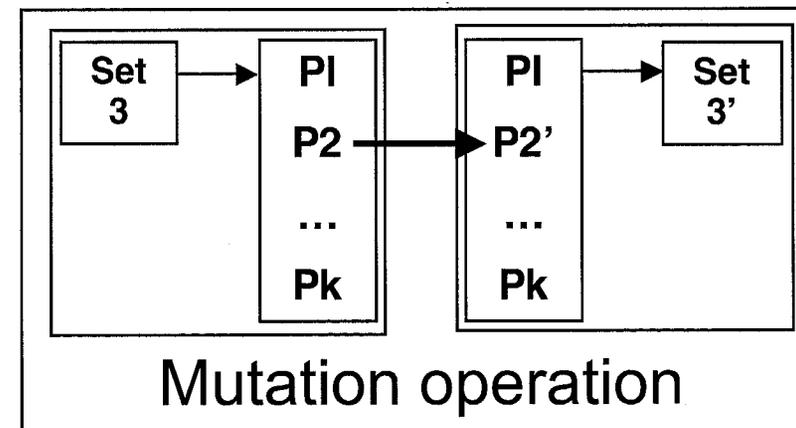
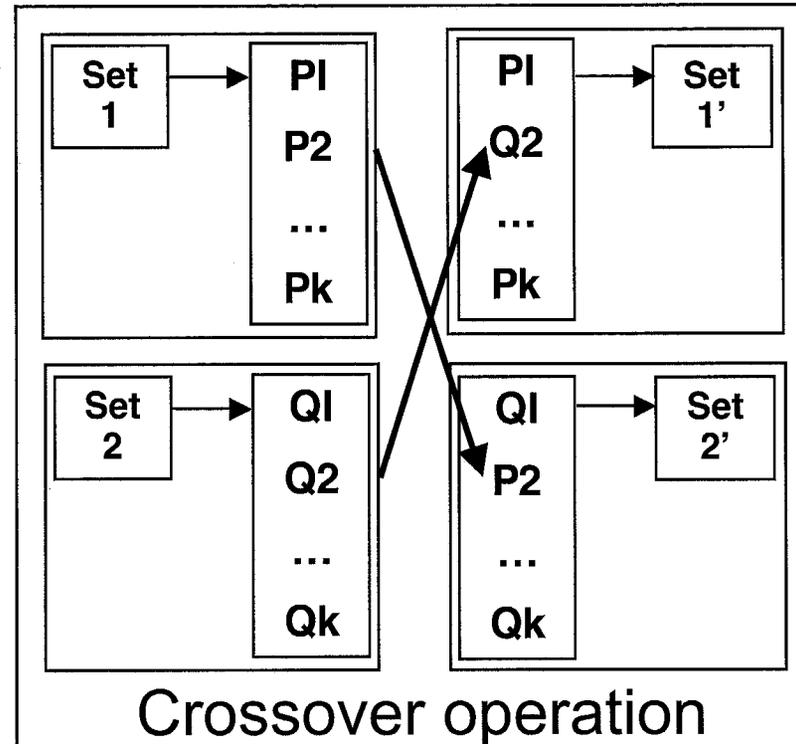
15-30 theoretical interaction energies

Genetic Algorithm



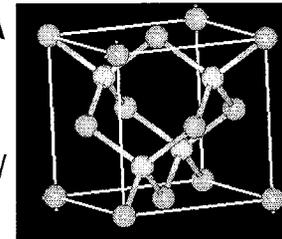
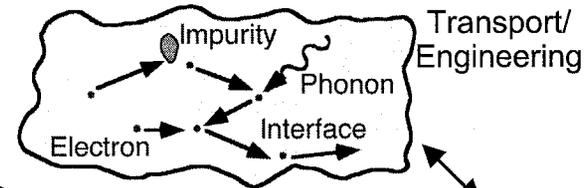
- Genetic algorithm parameter optimization is based on:
 - Survival of good parameter sets
 - Evolution of new parameter sets
 - Persistence of diversity (ensures global exploration)

- Basic Operations:
 - Crossover – gross exploration
 - Mutation – fine tuning



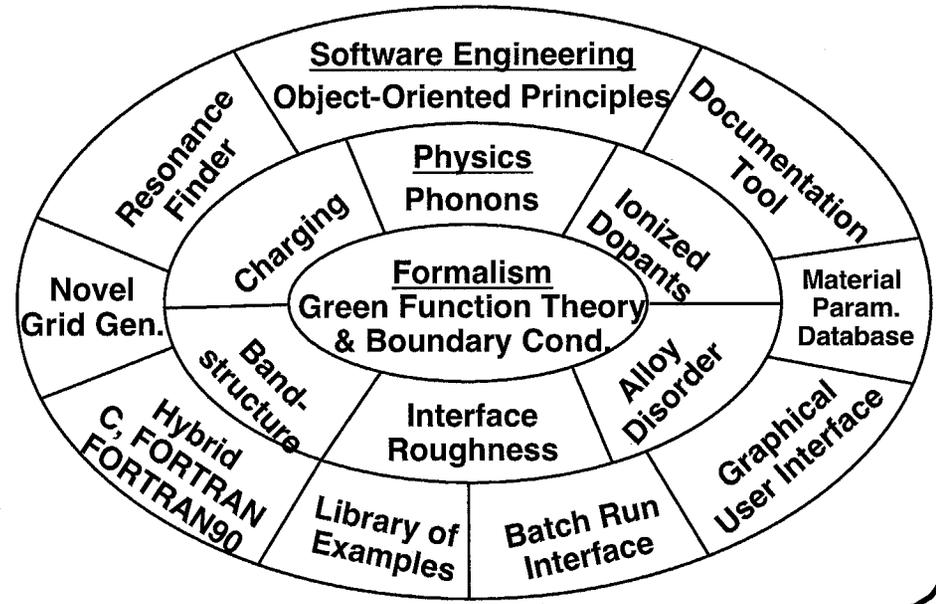
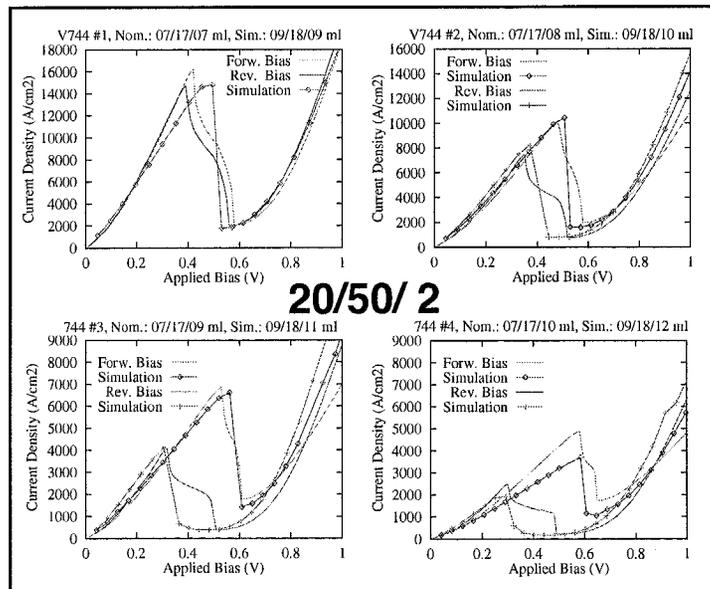
Leverage NEMO 1-D: A User-friendly Quantum Device Design Tool

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-97
 - >50,000 person hours of R&D
 - 250,000 lines of code in C, FORTRAN and F90
- Based on Non-Equilibrium Green function formalism (Datta, Lake, Klimeck).
- NEMO in THE state-of-the-art heterostructure design tool.
- Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.

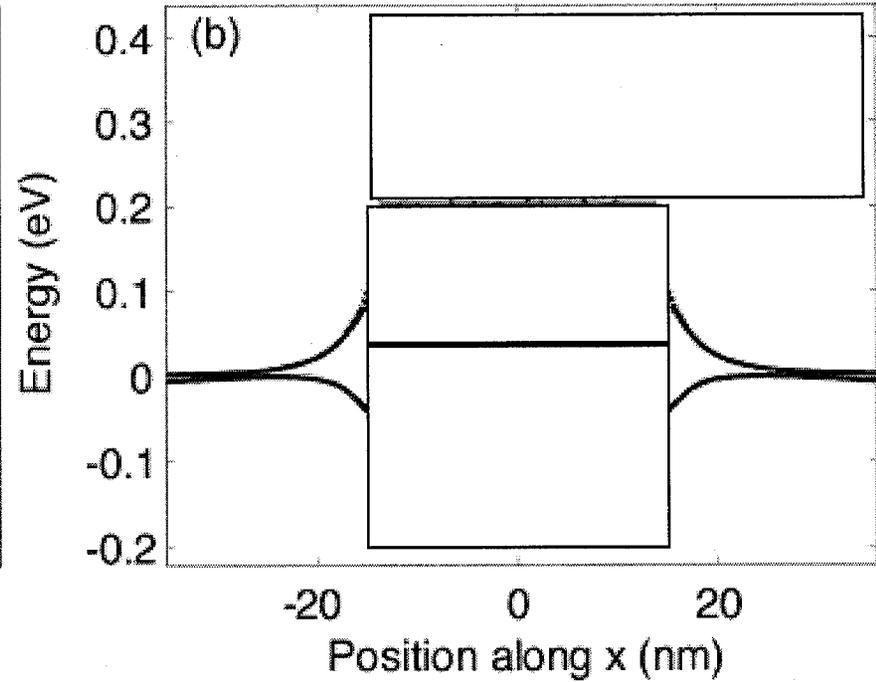
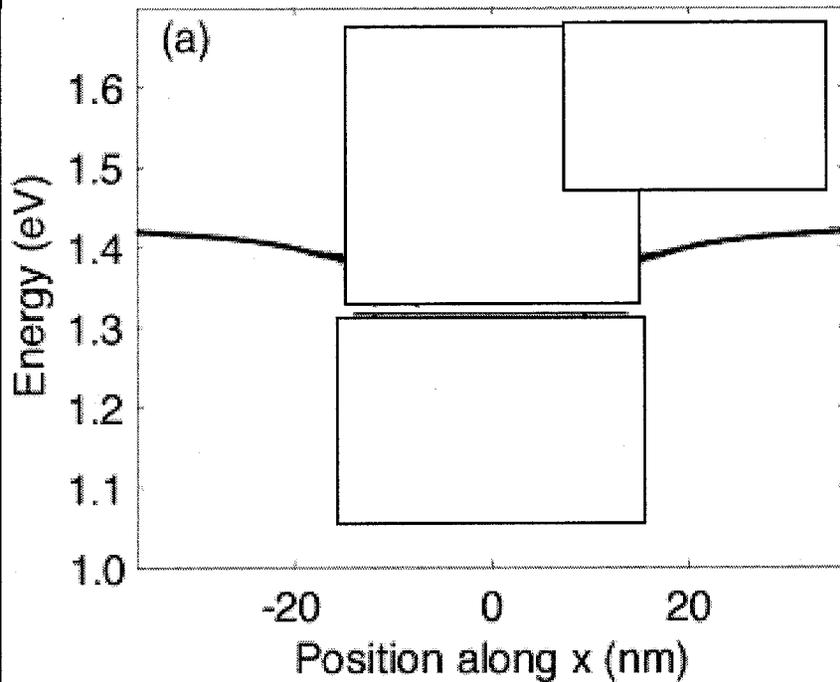


Quantum Mechanics / Physics

Testmatrix



Local Bandstructure in an Alloyed QD

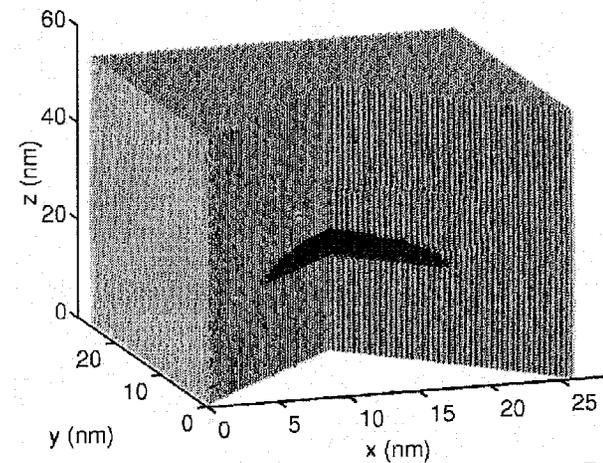


In-As bonds compressed in x-y

- > E_c raised from bulk value of $\sim 0.58\text{eV}$ to $\sim 1.2\text{eV}$
- > E_v HH raised from bulk value of $\sim 0.22\text{eV}$ to $\sim 0.3\text{eV}$

Ga-As bonds compressed in x-y and stretched in z

- > E_c raised from bulk value of $\sim 1.42\text{eV}$ to $\sim 1.55\text{eV}$
- > E_v raised from bulk value of 0eV to $\sim 0.1\text{eV}$



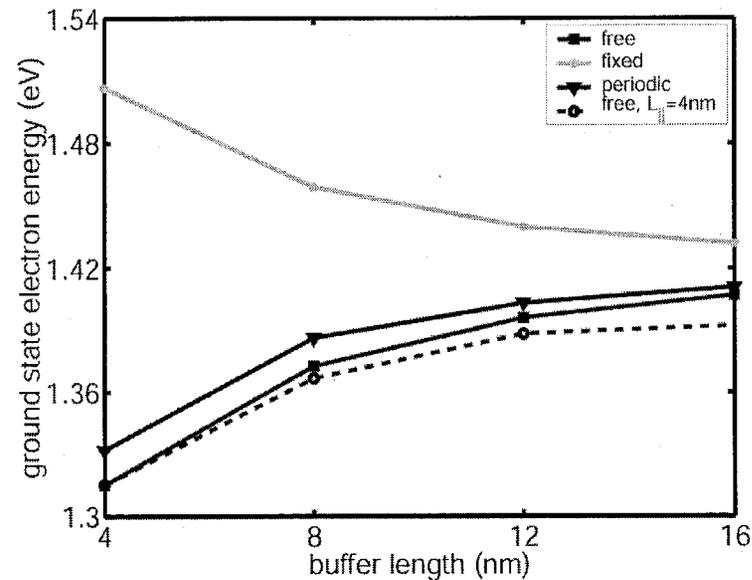
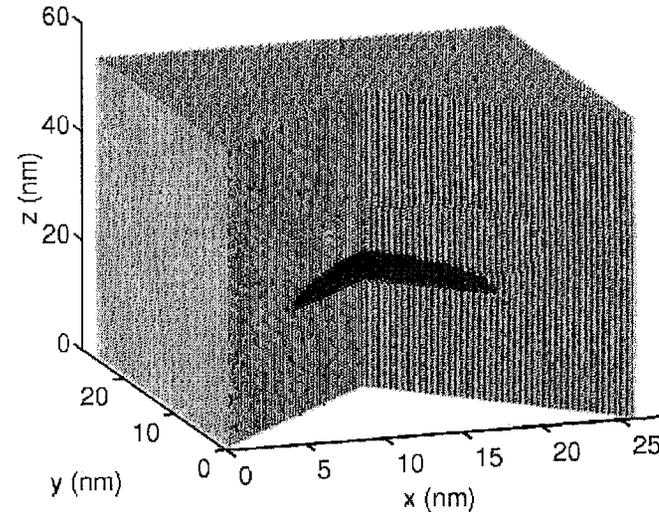
Issues with Boundary Conditions / System Size

Effect on ground state electron energy:

- System: Dome-shaped $\text{In}_{0.6}\text{Ga}_{0.4}\text{As}$ QD
15nm radius; 5.4 nm height
- **Free BC:** no constraints on QD; strain and ground state energy are underestimated
- **Fixed BC:** QD boundary pinned; strain and ground state energy are overestimated
- **Periodic BC** ($k_{\text{supercell}}=0$): Eigenvalues lie in between free and fixed case, but results are much closer to case of free BC.

Conclusions:

- Overall convergence is slow.
- Varying only vertical buffer size gives a good approximation.



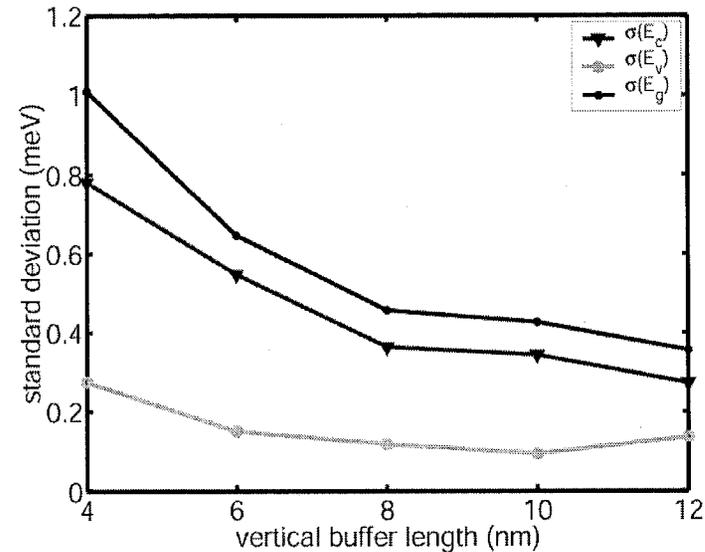
Disorder-induced Linewidth

Question: What is the contribution of alloy disorder to linewidth broadening?

- Previous PL experimental results have found large contributions due to inhomogeneous broadening (~ 30 meV) [R. Leon et al., PRB, 60, pR8517]
- Single QD PL measurements have found narrow linewidths (~ 0.9 meV) [Nagamune, APL, 67, p3257]

Computation:

- Use a 'direct sampling method' (roughly 100-200 samples)
- Assume no correlation between location of In, Ga cations within the QD



Results:

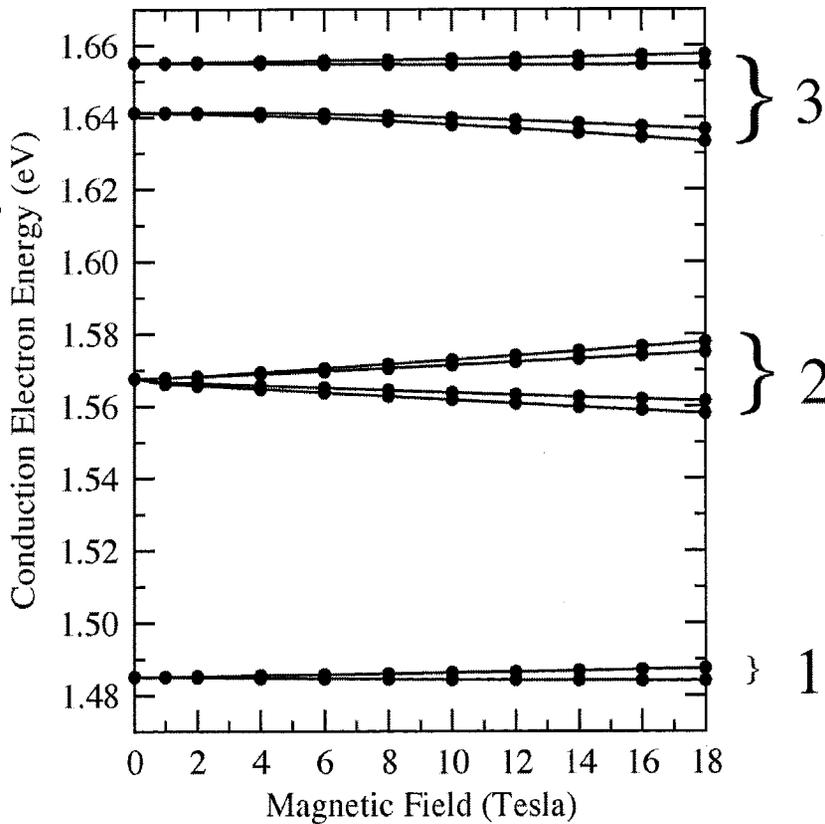
- Convergence is slow but can place an upper bound of 0.35 meV, so the effect is small.
- Caveats:
 - Have not included interface interdiffusion
 - Variation is larger if there is short-range order (clustering).

Magnetic-Field Effect on Electronic Structure of InAs Dot

(small dot on 2nm height and 10nm diameter, B field in growth direction)

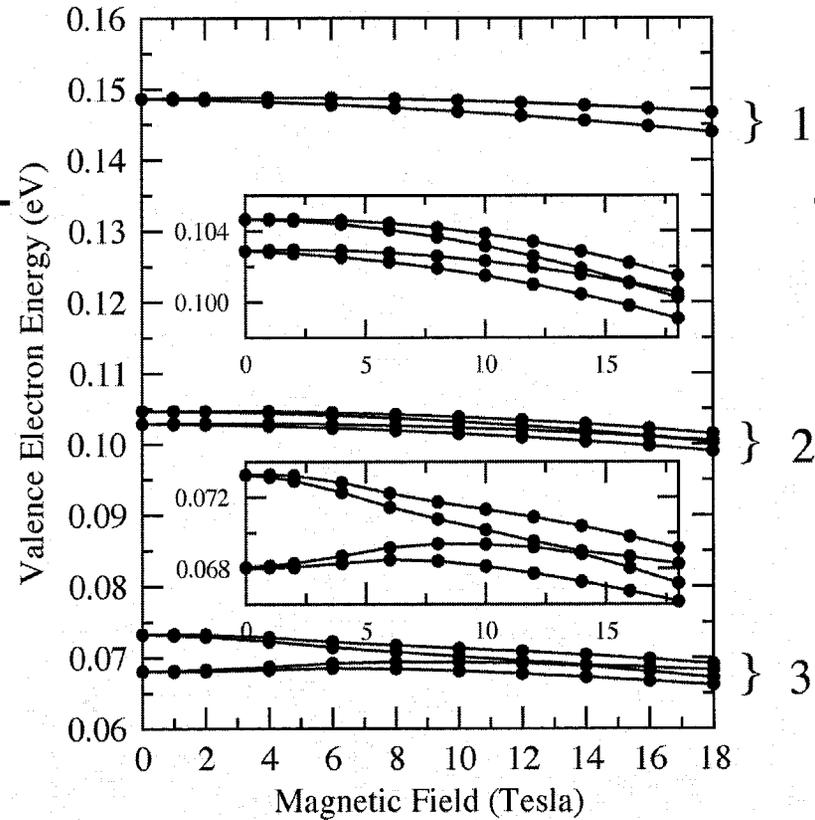
Conduction Electron Levels:

- Zeeman Interaction splits the levels into spin-up and -down levels.
- Effective g-factor ($g = (E_{\uparrow} - E_{\downarrow}) / \mu_B B$) ranges from 2 to 3.5.



Valence Electron Levels:

- Zeeman interaction splits the levels into $J_z = 3/2$ and $J_z = -3/2$ levels.
- Zeeman interaction couples closely-spaced levels.



Magneto-Optical Response of InAs Quantum Dot

Absorption Rate for Electron-Hole Pair Creation:

- Selective dipole coupling between electron and hole levels.
- The selectivity remains intact even at a high magnetic field because Zeeman interaction preserves the angular momentum of the level.

(Energy spacing of single electron states too large since quantum dot is small)

